Welcome to the Sixth Annual NASA Ames Research Center, Space Science and Astrobiology Jamboree at NASA Ames Research Center (ARC).

The Space Science and Astrobiology Division consists of over 60 Civil Servants, with more than 120 Cooperative Agreement Research Scientists, Post-Doctoral Fellows, Science Support Contractors, Visiting Scientists, and many other Research Associates.

Within the Division there is engagement in scientific investigations over a breadth of disciplines including Astrobiology, Astrophysics, Exobiology, Exoplanets, Planetary Systems Science, and many more. The Division's personnel support NASA spacecraft missions (current and planned), including SOFIA, K2, MSL, New Horizons, JWST, WFIRST, and others. Our top-notch science research staff is spread amongst three branches in five buildings at ARC. Naturally, it can thus be difficult to remain abreast of what fellow scientific researchers pursue actively, and then what may present and/or offer regarding inter-Branch, intra-Division future collaborative efforts. In organizing this annual jamboree, the goals are to offer a wholesome, one-venue opportunity to sense the active scientific research and spacecraft mission involvement within the Division; and to facilitate communication and collaboration amongst our research scientists.

Annually, the Division honors one senior research scientist with a Pollack Lecture, and one early-career research scientist with an Outstanding Early Career Space Scientist Lecture. For the Pollack Lecture, the honor is bestowed upon a senior researcher who has made significant contributions within any area of research aligned with space science and/or astrobiology. This year we are pleased to honor Linda Jahnke. With the Early Career Lecture, the honor is bestowed upon an early-career researcher who has substantially demonstrated great promise for significant contributions within space science, astrobiology, and/or, in support of spacecraft missions addressing such disciplines. This year we are pleased to honor Amanda Cook.

We hope that you will make time to join us for the day in meeting fellow Division members, expanding knowledge of our activities, and creating new collaborations within the Space Science and Astrobiology Division.

Sincerely Yours,

Jeffery Hollingsworth, SOC Lead
Steve Howell
Mark Fonda
Chris Dateo
Christine Martinez, LOC Lead

– The Science Organizing Committee of the Sixth Annual Code SS Science Jamboree

The Space Science and Astrobiology Division at NASA Ames Research Center would like to extend a thank you to all the contributors of this booklet as well as the various committees who worked behind the scenes to make this Jamboree event happen.

2018 Logistical Organizing Committee:
Christine Martinez , LOC Lead
Mojgan Momeni- Hassan
Taryn Kavanagh
Karina Shain
Lori Munar
Richard Nottage
Emmett Quigley

2018 Science Organizing Committee:
Jeff Hollingsworth, SOC Lead
Chris Dateo
Mark Fonda
Steve Howell

2018 Technical Support:
Chris Wilson
ACITS team

A special thank you to the building 3 staff at NASA Ames Research Center for your hospitality and planning support during this meeting.

SIXTH ANNUAL SPACE SCIENCE & ASTROBIOLOGY DIVISION SCIENCE JAMBOREE APRIL 4, 2018	
8:00 am	Registration & Poster Setup
Session Chair: Jeffery Hollingsworth	
8:30 am	Welcome & Announcements (Hollingsworth, Bicay)
8:45 am	***Outstanding Early Career Space Scientist Lecture:*** Amanda Cook: *Resource Prospector, Aeolus, and LADEE: Adventures of a Scientist in Mission Design and Science Instrumentation*
9:45 am	Dave Blake: *New Developments in X-Ray Diffraction for Planetary Exploration*
10:05 am	Melinda Kahre: *Recent Advances in Simulating the Martian Climate with the NASA Ames Mars Global Climate Model*
10:25 am	Poster Session (even number posters) & Coffee Break
Session Chair: Christopher Dateo	
11:10 am	Chris McKay: *Enceladus Life Signs and Habitability (ELSAH) Mission*
11:30 am	Ella Sciamma-O'Brien: *The Titan Haze Simulation Experiment: Dedicated Plasma Chemistry Model and Latest Laboratory Results*
11:50 am	Mary Beth Wilhelm: *Constraints on the Metabolic Activity of Microorganisms in Atacama Surface Soils Inferred from Refractory Biomarkers: Implications for Martian Habitability and Biomarker Detection*
12:10 pm	Poster Session / Lunch
Session Chair: Mark Fonda	
1:15 pm	Chris Materese: *Abiotic Synthesis of Nucleobases in Astrophysically Relevant Ices*
1:35 pm	Alessandra Ricca: *PAH Infrared Spectroscopy in the JWST Era: A Computational and Laboratory Study*
1:55 pm	Tim Lee: *Computing Highly Accurate Spectroscopic Line Lists for Characterization of Exoplanet Atmospheres and Assignment of Astronomical Observations*
2:15 pm	Niki Parenteau: *Examining the Evolution of Oxygenic Photosynthesis on the Early Earth and Potentially Exoplanets*
2:35 pm	Tom Roellig: *The Mid-Infrared Imager/Spectrometer/Coronagraph Instrument (MISC) for the Origins Space Telescope*
2:55 pm	Poster Session (odd number posters) & Coffee Break
Session Chair: Jeffery Hollingsworth	
3:40 pm	Pasquale Temi: *ARCUS – The X-Ray Grating Spectrometer Explorer*
4:00 pm	Joe Roser: *Ammonia on Charon: Laboratory Optical Constants of Ammonia Hydrates to Support New Horizons Observations*
4:20 pm	***Pollack Lecture:*** Linda Jahnke: *Biosignatures for Life Detection*
5:20 pm	Remove Posters

ID	Title	Corresponding Author
Astrobiology Posters		
AB.1	Enceladus Life Signs And Habitability (ELSAH) Mission	Chris Mckay
AB.2	Abiotic Synthesis of Nucleobases In Astrophysically Relevant Ices	Christopher Materese
AB.3	An Inventory of the Sugar Derivatives in Residues Produced from the UV Irradiation of Astrophysical Ice Analogs	Michel Nuevo
AB.4	Development of Microbial Platforms for High-Strength Polymers for Space and Earth Applications	Nils Averesch
AB.5	Engaging the Public with MarsFest Events in Death Valley National Park.	Rosalba Bonaccorsa
AB.6	Stanford-Brown iGEM 2017: Mars: Getting There and Staying There	Lynn Rothschild
AB.7	Constraints on the Metabolic Activity of Microorganisms in Atacama Surface Soils Inferred from Refractory Biomarkers: Implications for Martian Habitability and Biomarker Detection.	Mary Beth Wilhelm
AB.8	Testing Ice Collection For Europa & Enceladus Plume Fly-Through Missions.	David Willson
AB.9	New Developments In X-Ray Diffraction For Planetary Exploration.	David Blake
AB.10	Enantiomer Excesses In Meteoritic Organic Compounds: A Role For Radiation-Magnetism?	George Cooper
AB.11	An Astrobiology Outreach Activity: Meteorites, Organic molecules and the Origin of Life	Andro Rios/ George Cooper
AB.12	Circular Dichroism-Thermal Lens Microscopy: A New Approach to Life Detection	Hiroshi Imanaka
AB.13	Production And Preservation of Lipid Biomarkers By Iron-Oxidizing Chemolithotrophs In Circumneutral Iron Deposits	Niki Parentaeu
AB.14	Examining the Evolution of Oxygenic Photosynthesis on the Early Earth and Potentially Exoplanets	Niki Parentaeu
AB.15	The Impact of RNA Length on Evolution of RNA Function	Melina Popovich
AB.16	MAPX-PIXE: A Full Field Micro X-Ray Fluorescence Imager for Astrobiology Applications on Ocean Worlds.	Richard Walroth
AB.17	Novel Possibilities in Material Extraction Enabled Through Biological In Situ Resource Utilization (ISRU)	Benjamin Lehner
Astrophysics Posters		
AP.1	An HI Survey of Extremely Isolated Early-type Galaxies	Trisha Ashley
AP.2	Dynamics of Pure and N-substituted Cyclic Aromatic Hydrocarbon Formation in the Gas-Phase	Partha Bera
AP.3	Tracing the Charge Balance of Polycyclic Aromatic Hydrocarbons Across a Reflection Nebula, an H II-Region and a Planetary Nebula	Christiaan Boersma
AP.4	Inferring Fundamental Properties of Young Stars and Brown Dwarfs	Michael Gully-Santiago
AP.5	PAH Infrared Spectroscopy in the JWST Era: a Computational and	Alessandra Ricca

	Laboratory Study	
AP.6	The Mid-Infrared Imager/Spectrometer/Coronagraph Instrument (MISC) for the Origins Space Telescope	Tom Roellig
AP.7	The COsmic SImulation Chamber (COSmIC) at NASA Ames: a Multipurpose Laboratory Astrophysics Facility	Farid Salama
AP.8	The Astronomical 7.7 μm Polycyclic Aromatic Hydrocarbon Complex: Insights from the NASA Ames PAH Infrared Spectroscopic Database	Matthew Shannon
AP.9	Shaken Snow Globes: Kinematic Tracers of the Multiphase Condensation Cascade in Massive Galaxies	Pasquale Temi
AP.10	ALMA Observations of Molecular Clouds in Three Group Centered Elliptical Galaxies	Pasquale Temi
AP.11	Arcus - The X-ray Grating Spectrometer Explorer	Pasquale Temi
Exoplanet Posters		
EP.1	A Survey Astronomy Laboratory Sequence Covering Exoplanets	Michael Fanelli
EP.2	Computing Highly Accurate Spectroscopic Line Lists for Characterization of Exoplanet Atmospheres and Assignment of Astronomical Observations	Tim Lee
EP.3	Limits On Undetected Planets in the Six Transiting Planets Kepler-11 System	Jack Lissauer
EP.4	Using Final Kepler Catalog Completeness and Reliability Products in Exoplanet Occurance Rate Estimates	Steve Bryson
Ep.5	The Transiting Exoplanet Community Early Release Science Program for JWST.	Natalie Batalha
Planetary Atmosphere and Climate		
PA.1	Aeolus: A Mission to Study the Winds and Climate of Mars.	Amanda Cook
PA.2	The Titan Haze Simulation Experiment: Dedicated Plasma Chemistry Model and Latest Laboratory Results	Ella Sciamma O' Brien
PA.3	Detecting Secular Climate Change on Mars: An Update	Courtney Batterson
PA.4	Investigating the Closure of the Dust Cycle on Current Mars by Implementing the Tagging Method in the NASA Ames MGCM	Tanguy Bertrand
PA.5	The Latest on the Venus Thermospheric General Circulation Model: Capabilities and Simulations	Amanda Brecht
PA.6	Maintenance of Background Dust Opacity with Wind Stress Based Dust Lifting During Northern Hemisphere Summer on Mars.	Vandana Jha
PA.7	Recent Advances in Simulating the Martian Climate with the NASA Ames Mars Global Climate Model	Melinda Khare
PA.8	Modularization in the Ames Mars General Circulation Model Ecosystem	Richard Urata
PA.9	Assessing Atmospheric Thermal Forcing From Surface Pressure Data: Separating Thermal Tides and Local Topographic Influence	John Wilson
PA.10	Beyond Mie Theory: Scattering by Spheroidal Particles	Sanford Davis

Planetary Surfaces & Interiors		
PS.1	Micro-CT Analysis Of Meteorite Flaws And Scaling For Asteroid Atmospheric Entry	Kathryn Bryson
PS.2	Ammonia on Charon: Laboratory Optical Constants of Ammonia Hydrates to Support New Horizons Observations	Joe Roser
PS.3	High Temperature Emissivity Of Meteorites Related To Asteroid Atmospheric Entry	Daniel Ostrowski
PS.4	Using Satellite Data to Differentiate between Rock and Regolith on Earth's Surface	Corina Cerovski-Darriau and Jonathan Stock

Outstanding Early Career Space Science Lecture: Amanda Cook

8:45am

Resource Prospector, Aeolus, and LADEE: Adventures of a Scientist in Mission Design and Science Instrumentation

Amanda Cook

Abstract:
In this talk, Dr. Cook will devote primary focus to the Resource Prospector and Aeolus missions, and touch on her work with O/OREOS and LADEE (Lunar and Dust Environment Explorer). Resource Prospector (RP) is a rover mission to the lunar poles, currently aiming for launch in the early 2020s. The mission will prospect and drill, looking for water and OH near the poles and in permanently shadowed regions. The RP payload includes the Near-IR Volatile Spectrometer System (NIRVSS), for which Amanda serves as the Integration and Test and Operations lead.

Aeolus is a mission concept to directly measure the winds and climate of Mars, by measuring surface and atmospheric temperatures, aerosol abundances, and Doppler shifts in atmospheric spectral lines. Aeolus objectives are to: (1) Characterize Mars global circulation processes, including seasonal and diurnal changes, (2) determine the relative contributions to the global energy balance at Mars by measuring rejected solar radiation, and thermal emission from the Martian surface and atmosphere, and (3) measure Martian atmospheric aerosol (H_2O ice, dust) distribution.

Lastly, starting in 2016, Amanda began work with the Ames Mission Design Center to formalize a process for developing science concepts into mission designs using Concept Maturity Levels (similar to Technical Readiness Levels, but for developing mission concepts). The goal was to create a roadmap for interested PIs to engage with the Mission Design Center from the earliest formulation phases of their brainstorming to the production of an extended report that outlines the feasibility and estimated cost of the concept. Amanda will discuss this new process to highlight how scientists at Ames can get involved with the formulation of new missions.

NEW DEVELOPMENTS IN X-RAY DIFFRACTION FOR PLANETARY EXPLORATION. D. Blake[1], P. Sarrazin[2], M. Gailhanou[3], J. Chen[4], P. Dera[5], B. Downs[6], R. Walroth[1] and T. Bristow[1], [1] Exobiology Branch, NASA Ames Research Center, Moffett Field, CA 94035, [2] SETI Institute, Mountain View, CA 94043, [3] CNRS, IM2NP UMR, Marseille, France, [4] Baja Technology, Tempe, AZ, [5] HIGP, Univ. of Hawai'i, Honolulu, HI, [6] Geosciences, Univ. Arizona, Tucson AZ 85721-0077.

Introduction: X-ray diffraction (XRD) is the gold standard for definitive, quantitative mineralogical analysis. The MSL CheMin instrument established the quantitative mineralogy of the Mars soil [1], characterized the first habitable environment on another planet [2], and provided the first *in-situ* evidence of Martian silicic volcanism [3]. CheMin is now characterizing lacustrine mudstones that comprise the lower strata of Mt. Sharp [4] that contain evidence of the gradual dessication and oxidation of the Mars surface.

Even with its simplified sample movement system, CheMin still requires substantial sample preparation. Deployment of XRDs on smaller missions will require simplified sample preparation, decreased instrument size and complexity, and improved 2θ resolution. Efforts in these directions are underway.

XRD with Limited Sample Preparation: XTRA (Extraterrestrial Regolith Analyzer) will analyze fines in as-delivered surface regolith [5]. Fine-grained regolith coats the surfaces of most airless bodies in the solar system, and can often be used as a proxy for the surface mineralogy. XTRA can be configured in transmission or reflection geometry using vibrated cells for as-delivered powders, allowing direct analysis of materials scooped at the surface.

XRD without Sample Preparation: Hybrid-XRD (HXRD) is concept under development to analyze rocks or soils without sample preparation [6]. If the material is sufficiently fine-grained, a powder XRD pattern is obtained, similar to CheMin or XTRA. With coarse-grained crystals, the white bremsstrahlung radiation of the tube is diffracted into single crystal Laue patterns. Unlike typical Laue applications, HXRD analyzes the energy of each Laue spot, enabling the measurement of single crystal Bragg diffractions. Dedicated crystallographic software has been developed for identification of minerals responsible for the Laue patterns.

High resolution XRD: With CheMin and any of the previously described XRD concepts, instrument resolution suffers from system miniaturization and is limited to about 0.3°2θ. A planetary XRD based on Guinier geometry is under development to provide a compact high-resolution instrument. A substantial gain in resolution has been demonstrated with a basic proof-of-concept instrument. Both reflection and transmission geometries can be developed with the Guinier design and are being explored as part of a PICASSO funded project.

Development of High TRL Components: High TRL subsystems are being developed for future XRD instruments. Special CCD detectors are being developed with e2V (UK (Fig. 1A). Custom FPGA based electronics for low noise CCD operation with embedded data processing capabilities are under development with Baja Technology (Fig. 1B). Miniature X-ray tubes are being developed in collaboration with RTW of Germany (Fig. 1C) that are compatible with power supplies developed by Battel Engineering (Fig. 1D).

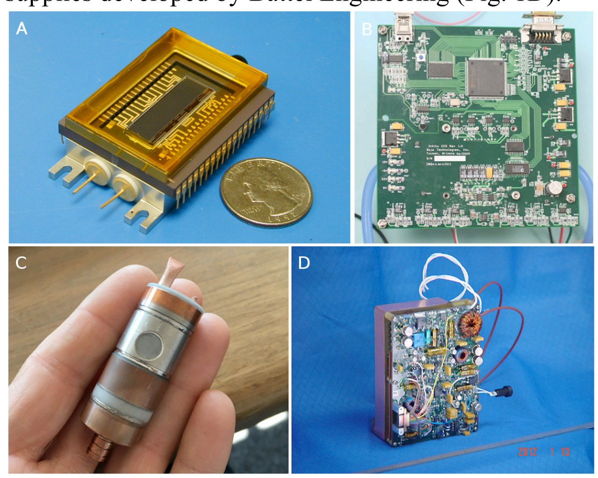


Fig 1: Example of flight components under development with industrial partners: A. X-ray CCD in flight package with internal peltier cooler (e2V); B. CCD control electronics (Baja Technologies); C. Miniature microfocused X-ray tube (RTW); D. X-ray tube power module with HVPS stage (Battel Engineering).

Deployment Opportunities: Future instruments proposed for flight will be tailored to the specific mission constraints and will be comprised of combinations of the features and flight hardware presented above.

References:

[1] *Science,* 341, 1238932; doi:10.1126/science.1238932, [2] *Science*, 10.1126/science.1243480. [3] PNAS: doi: 10.1073/pnas.1607098113 [4] *Science,* 356 eaah6849 DOI:10.1126/science.aah6849 [5] IEEE Aerospace Conference, Big Sky, MO, March, 2012. Paper #2.0905 [6] LPSC 40 #1496.

Acknowledgements: The authors are grateful for support from NASA/ARC's Center Innovation Fund and NASA's PICASSO program (grant # NNX15AM95G).

Title: Recent Advances in Simulating the Martian Climate with the NASA Ames Mars Global Climate Model

Authors: Melinda A. Kahre, Jeffery L. Hollingsworth, R. John Wilson, Robert M. Haberle, Amanda S. Brecht, Richard A. Urata, Alex Kling, Vandana Jha, Courtney M. Batterson, Tanguy Bertrand, and Kathryn E. Steakley

Science Topic: Planetary Atmosphere & Climate

NASA's Mars Climate Modeling Center at Ames Research Center is currently undergoing an exciting period of growth in personnel, modeling capabilities, and science productivity. We are transitioning from our legacy C-grid finite-difference dynamical core to the NOAA/GFDL cubed-sphere finite-volume (FV3) dynamical core for simulating the climate of Mars (Figure 1). This highly parallelized core is scalable and flexible, which will allow for significant improvements in the horizontal resolution of our simulations. We are currently porting the Mars-specific physical process codes developed here at Ames over the past several decades into the new dynamical core. In addition to this new model development, our group has made progress advancing our understanding of the current and past climate of Mars. We have addressed many questions regarding the current CO_2, dust and water cycles and the dynamical processes that control them. Further, we have begun investigations into the photochemistry and transport processes of the upper atmosphere. Finally, we have initiated studies of the climate systems of the Amazonian, Hesperian, and Noachian periods of Martian history. We will present these new model capabilities and insights into the atmosphere and climate of Mars.

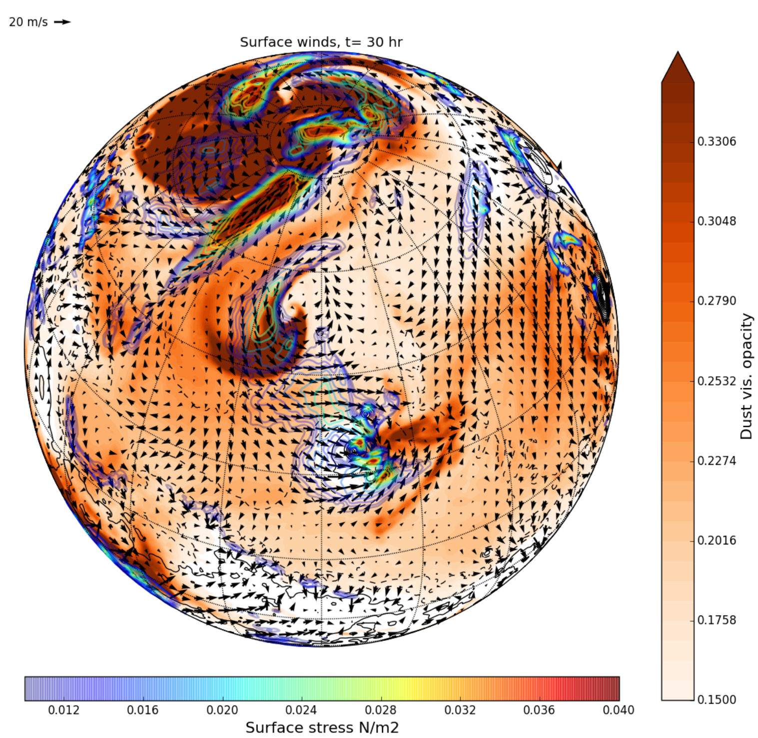


Figure 1: Column dust opacity (shading), surface wind stress (contours) and low-level winds (vectors) from a high-resolution simulation with the NASA Ames Mars GCM that features a new dynamical core. Wind vectors are subsampled for clarity. These instantaneous fields are from an animation used to explore interactions between dust lifting, dust transport, and the general circulation.

Oral Presentation: **11:10am**

Enceladus Life Signs And Habitability (ELSAH) mission

Chris McKay, Alfonso Davila, Jen Heldmann, Richard Quinn, Tori Hoehler, Niki Parenteau, Tony Ricco, Carol Stoker, David Willson (The members of the ELSAH Development Team at NASA Ames).

ELSAH is a mission to explore and sample the plume of material emerging from Enceladus' South Polar Terrain. Its science goals are to search for biosignatures in the plume, assess the habitability of Enceladus' subsurface ocean, and to examine the plume's overall structure and dynamics. The goals of identifying biosignatures and assessing habitability will be addressed using two in-situ instruments: a mass spectrometer called PALMS and a wet chemistry lab system called µCAFÉ. These instruments will receive particle and gaseous material from the plume and examine various chemical indicators of habitable environments and life, including redox state, distributions and chirality of amino acids, and distributions of fatty acids. These instruments will sample the plume over a series of flybys where the spacecraft flies through the base of the plume at low (<1.5 km/s) encounter speeds. The goal of characterizing the moon's overall activity will be addressed by two remote-sensing instruments, a visible camera called NAC and a thermal infrared instrument called ENTIR. NAC will observe the plume prior to the first close encounter in order to characterize Enceladus' activity, while both ENTIR and NAC will map the South Polar Terrain during each flyby to identify sources and characterize their geological context.

The Titan Haze Simulation Experiment: Dedicated Plasma Chemistry Model and Latest Laboratory Results

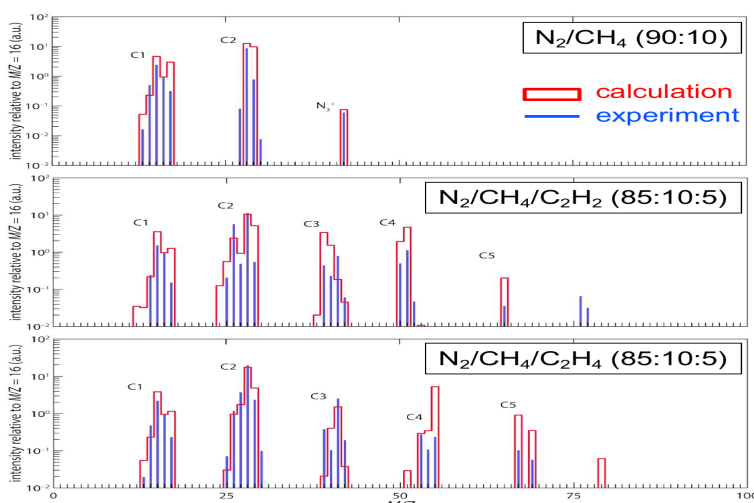
Sciamma-O'Brien E.[1, 2], Raymond A. W.[3], Upton K. T.[4], Mazur E.[3], Salama F.[1]
[1]NASA Ames Research Center, Moffett Field, CA, USA,[2]Bay Area Environmental Research Institute, Moffett Field, CA, USA [3]Harvard University, Cambridge, MA, USA, [4]Indiana University Bloomington, IN, USA

Science Topic: Planetary Atmosphere & Climate

The Titan Haze Simulation (THS) experiment, developed at the NASA Ames COSmIC simulation chamber is a unique experimental platform that allows us to simulate Titan's complex atmospheric chemistry at Titan-like temperature (200 K) by cooling down N_2-CH_4-based mixtures in a supersonic expansion before inducing the chemistry by plasma. Both the gas and solid phase can be characterized.

Because of the accelerated gas flow in the expansion, the residence time of the gas in the active plasma region is less than 4 μs. This results in a truncated chemistry that enables us to control how far in the chain of chemical reactions the chemistry is processing, by adding, in the initial gas mixture, heavier molecules that have been detected as trace elements on Titan (Sciamma-O'Brien et al., 2014). This unique aspect of the THS has been confirmed by a new model developed to simulate the plasma chemistry in the THS, and which follows the evolution in time and space of more than 120 species using electron impact and chemical kinetics equations. The calculated mass spectra are in good agreement with the experimental THS mass spectra, confirming that the short residence time in the plasma cavity limits the growth of larger species (Raymond et al., 2018).

The THS solid phase component has also been characterized using scanning electron microscopy, infrared spectroscopy and x-ray absorption spectroscopy that have shown differences in the morphology of the grains produced as well as differences in the level and nature of the nitrogen incorporation depending on the composition of the initial gas mixture. A comparison to Cassini VIMS observational data has shown that the THS aerosols produced in simpler mixtures, i.e., that contain more nitrogen and where the N-incorporation is in isocyanide-type molecules instead of nitriles, are more representative of Titan's aerosols (Sciamma-O'Brien et al., 2017). In the next step in the analysis of the THS aerosols, a study will be initiated to determine their optical constants from the UV to the Far IR using a new optical constant facility that has recently been added.



References:
Sciamma-O'Brien E., Ricketts C.L. and Salama F.., Icarus, 243, 325 (2014)
Sciamma-O'Brien E., Upton K. and Salama F., Icarus, 289, 214 (2017)
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Acknowledgements: This research is supported by the SSW Program of NASA SMD and a SERA. The authors acknowledge the technical support of E. Quigley.

Constraints on the Metabolic Activity of Microorganisms in Atacama Surface Soils Inferred from Refractory Biomarkers: Implications for Martian Habitability and Biomarker Detection.

Mary Beth Wilhelm[1,2,], Alfonso F. Davila[1] , Mary N. Parenteau[1], Linda L. Jahnke[1], Mastewal Abate[1], George Cooper[1], E. Taylor Kelly[3], Victor Parro García[4], Miriam G. Villadangos[4], Yolanda Blanco [4], Brian Glass[5], James J. Wray[2], Jennifer L. Eigenbrode[6], Roger E. Summons[7], Kimberly Warren-Rhodes[3]

[1]Space Science and Astrobiology Division, NASA Ames Research Center; [2]School of Earth and Atmospheric Sciences, Georgia Institute of Technology; [3]Carl Sagan Center, SETI Institute; [4]Departamento Evolución Molecular, Centro de Astrobiologia (INTA-CSIC), Madrid, Spain; [5]Intelligent Systems Division, NASA Ames; [6]Planetary Environments Laboratory, NASA Goddard; [7]Department of Earth, Atmospheric, and Planetary Sciences, Massachusetts Institute of Technology

Abstract: Dryness is one of the main environmental challenges to microbial survival. Understanding the threshold of microbial tolerance to extreme dryness is relevant to better constrain the environmental limits of life on Earth, and also to critically evaluate long-term habitability models of Mars. Biomolecular proxies for microbial adaptation and growth were measured in Mars-like hyperarid surface soils in the Atacama Desert that experience only few millimeters of precipitation per decade, and in biologically active soils a few hundred kilometers away that experience 2-5 fold more precipitation. Diversity and abundance of lipids and other biomolecules decreased with increasing dryness. Cyclopropane fatty acids (CFA), indicative of adaptive response to environmental stress and growth in bacteria, were only detected in the wetter surface soils. The ratio of *trans* to *cis* isomers of an unsaturated fatty acid, another bacterial stress indicator, decreased with increasingly dry conditions. Aspartic acid racemization ratios increased from 0.01 in the wetter soils to 0.1 in the driest soils, indicative of racemization rates comparable to *de novo* biosynthesis over long time scales (~10,000 years). The content and integrity of stress proteins profiled by immunoassays were additional indicators that biomass in the driest soils is not recycled at significant levels. Together, our results point to minimal or no *in situ* microbial growth in the driest surface soils of the Atacama, and any metabolic activity is likely to be basal, for cellular repair and maintenance only. Our data add to a growing body of evidence that the driest Atacama surface soils represent a threshold for long-term habitability (i.e., growth and reproduction). These results place constraints on the potential for extant life on the surface of Mars, which is 100-1000 times drier than the driest regions in the Atacama.

ABIOTIC SYNTHESIS OF NUCLEOBASES IN ASTROPHYSICALLY RELEVANT ICES.
C. K. Materese[1,2], M. Nuevo[1,2], P.P. Bera[1,2], T.J. Lee[1] and S. A. Sandford[1], [1]NASA Ames Research Center, Moffett Field, CA, USA, [2]BAER Institute, Moffett Field, CA, USA

Introduction: Nucleobases are biomolecules that act as the fundamental components of the alphabet from which known life is encoded (Fig. 1). They are highly conserved between species and were likely important during the early emergence of life. To date, no experimental conditions have been determined that could abiotically produce all of the primary biological nucleobases in a terrestrial environment or in an early terrestrial analog.

We have demonstrated, experimentally and computationally, that it is possible to produce all of the biological nucleobases from the UV-irradiation of pyrimidine and purine in simple astrophysical ice analogs [1-7]. Here we present a full summary of the results of all of our efforts on this topic.

Experimental: Volatile gases were premixed in ~2L bulbs which were attached to a cryogenic vacuum chamber. Purine was prepared separately in an evacuated sample tube that was attached directly to the vacuum chamber, and wrapped with heat tape and a thermocouple to control and monitor the temperature and deposition rate. Reactants were vapor deposited onto a cooled substrate in the vacuum chamber that maintained a temperature of ~15K. Throughout deposition, the ice were simultaneously irradiated with an H_2-discharge lamp emitting UV photons (Lyman α at 121.6 nm and a continuum centered at ~160 nm). After irradiation, samples were warmed to room temperature, and refractory residues were recovered for derivatization and analysis.

Computational: Structures and energies of the reactants, intermediates, and products along the reaction path were calculated using modern range-separated hybrid meta-GGA (wB97M-V) density functional methods (DFT) along with large basis sets for both gas phase as well as condensed phase conditions. The effects of the extended ice environment were modeled by a conductor-like polarized continuum model (C-PCM) in which the bulk is represented as a polizable medium characterized by its dielectric constant.

Results: Our work has demonstrated that the UV-photoirradiation of pyrimidine and purine in astrophypsical ice analogs leads to the production of all of the primary nucleobases, and numerous other compounds of potential prebiotic interest. The relative abundances of these compounds is heavily dependent on the following: 1) The composition of the starting ice mixture, which impacts the type of functional groups available for substitution, the proton affinity of the surroundings, the UV-cross section, and the number of species in competition for substitution; 2) the number of functional group additions required to form the product. More substitutions requires more photons and more potential ways for the production pathway to be disrupted; 3) The type of functional group added to pyrimidine or purine. Functional groups are produced with different efficiencies from the reactant ices and the energetic favorability of their additions to pyrimidine or purine plays a role; 4) The position where the addition takes place is also important for both energetic (e.g. ease of deprotonation) and statistical reasons (e.g. numerous ways to produce identical isomers).

The ice matrix plays very important, and sometimes contradictory, roles as a medium for reaction, and as a progenitor of ions. The mechanisms involving a cationic route dominate. The gas phase mechanism of formation of nucleobasee is ineffective, and the presence of condensed phase is necessary.

Conclusion: Our results demonstrate that all biological nucleobases can be produced under similar astrophysical conditions. These nucleobases and other pyrimidine and purine derivatives are produced with large differences in their relative abundances. If compounds of astrophysical origin are important for the emergence of life, our results suggest that some nucleobases (uracil, cytosine, and adenine) were far more abundant than others (thymine and guanine) and may suggest that some alternative compounds (e.g. hypoxanthine, a guanine substitute) may have played roles early in the evolution of life.

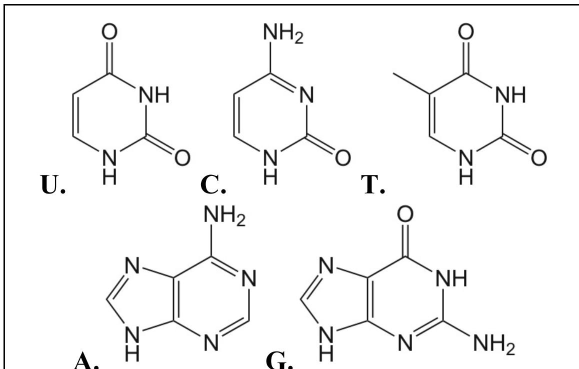


Fig. 1. The five primary biological nucleobases. **U.** Uracil **C.** Cytosine **T.** Thymine **A.** Adenine **G.** Guanine

References: [1] Nuevo M. et al. (2009) *Astrobiology,* 9, 683. [2] Bera P. P. et al. (2010) *JCP*, 133, 104303 [3] Nuevo M. et al. (2012) *Astrobiology,* 12, 295. [4] Materese C. K. et al. (2013) *Astrobiology,* 13, 948. [5] Nuevo M. et al. (2014) *ApJ*, 793, 125. Bera P. P. et al. (2016) *JCP,* 144, 144308. [6] Materese C. K. et al. (2017) *Astrobiology,* 17, 761. [7] Bera P. P. et al. (2017) *Astrobiology,* 17, 771.

Oral Presentation: 1:35pm

PAH Infrared Spectroscopy in the JWST Era: a computational and laboratory study

Authors: Alessandra Ricca[1,2], Joseph Roser[1,2], Jean Chiar[1,3], Els Peeters[4], Xander Tielens[5]
Affiliations: (1) SETI Institute (2) NASA-Ames Research Center (3) Diablo Valley College (4) University of Western Ontario, Canada (5) Leiden University

Abstract: The Infrared Space Observatory and Spitzer Space Telescopes have shown that the mid-IR emission spectrum of the interstellar medium is dominated by strong bands at 3.3, 6.2, 7.7, 8.6, 11.3 and 12.7 microns superimposed upon broad underlying plateaus generally attributed to PAHs, PAH clusters and very small grains. Despite the limited spectral and spatial resolution of these data, detailed analysis has revealed that each band is, in fact, a blend of multiple emission features. Subtle variations in the band blending can be detected even for spectra measured at different positions within a single astronomical source. These variations can be seen to arise from multiple PAH and PAH-related carriers that are each responding differently to the local physical conditions. The James Webb Space Telescope has near-IR and mid-IR instruments, NIRSpec and MIRI, with an extremely high spectral resolution, spatial resolution, and sensitivity that will revolutionize infrared astronomy. These instruments will provide spatial maps on a sub-arcsecond scale with an unprecedented level of spectral detail, allowing detailed study of the interrelationship of the individual components within each emission band. This will provide a critical insight into the molecular characteristics of the emitting species and their (photo)chemical evolution in space.

Exploitation of these astronomical spectra requires infrared data on potential emitting species that fully account for all astrophysically relevant materials. We have undertaken a combined program of computational modeling and laboratory experiments to be conducted at NASA-Ames Research Center to calculate the IR spectra of isolated as well as clustered neutral and charged PAHs containing up to 150 carbon atoms and with a wide variety of structures ranging from compact with straight edges, compact with bay regions, non-compact with various shapes and erosion sites, and PAHs containing defects. These theoretical data are be validated by a dedicated laboratory study of neutral and cationic PAH species containing up to 70 carbon atoms and their clusters. The IR absorption spectra are used to calculate emission spectra that can be directly compared to existing Spitzer Infrared Spectrograph (IRS) maps of reflection nebulae (RNe) and star forming regions and future astronomical observations obtained by NIRSpec and MIRI on JWST, as shown in Figure 1.

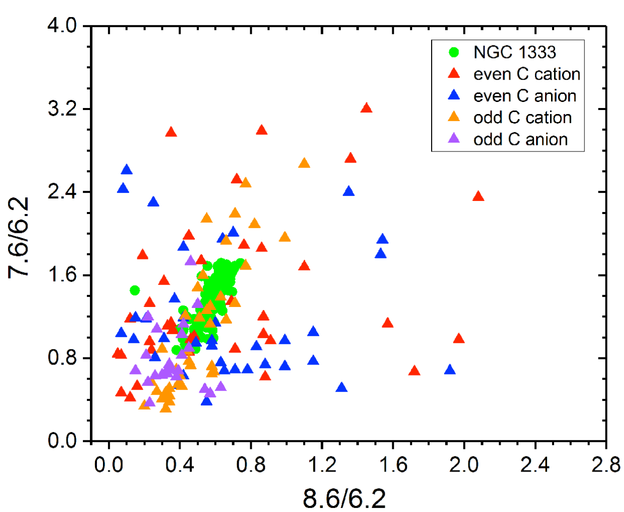


Figure 1. Comparison of the intensity ratios of even-carbon PAH cations (red triangles) and anions (blue triangles), and odd-carbon PAH cations (orange triangles) and anions (purple triangles), computed for an excitation of 8 eV and after applying a redshift of 15 cm^{-1}, with observations (green circles) of the RNe NGC 1333.

Computing highly accurate spectroscopic line lists for characterization of exoplanet atmospheres and assignment of astronomical observations

Timothy J. Lee[a], **Xinchuan Huang**[a,b], **and David W. Schwenke**[c]
[a]Space Science & Astrobiology Division, NASA Ames Res. Ctr., Moffett Field, CA, USA
[b]SETI Institute, Mountain View CA, USA
[c]NAS Facility, NASA Ames Research Center, Moffett Field, CA, USA

Over the last decade, it has become apparent that the most effective approach for determining highly accurate rotational and rovibrational line lists for molecules of interest in planetary atmospheres and other astrophysical environments is through a combination of high-resolution laboratory experiments coupled with state-of-the art *ab initio* quantum chemistry methods. The approach involves computing the most accurate potential energy surface (PES) possible using state-of-the art electronic structure methods, followed by computing rotational and rovibrational energy levels using an exact variational method to solve the nuclear Schrödinger equation. Then, reliable experimental data from high-resolution experiments is used to refine the *ab initio* PES in order to improve the accuracy of the computed energy levels and transition energies. From the refinement step, we have been able to achieve an accuracy of approximately σ_{RMS}= 0.02 cm^{-1} for rovibrational transition energies, and even better for purely rotational transitions. This combined "experiment + theory" approach allows for determination of essentially a complete line list, with hundreds of millions of transitions, and having the transition energies and intensities be highly accurate. Our group has successfully applied this approach to determine highly accurate line lists for NH_3 and CO_2 (and isotopologues), and very recently for SO_2 and isotopologues. Here I will report our latest results for SO_2 isotopologues and updates on CO_2 isotopologues. Comparisons to the available data in HITRAN2016 and other available experimental data will be shown, though we note that our line lists for SO_2 isotopologues are significantly more complete than any other databases. Since it is important to span a large temperature range in order to model the spectral signature of exoplanets, we will also demonstrate how the spectra of CO_2 change on going from low temperatures (100 K) to higher temperatures (500 K to 1500 K).

Oral Presentation: **2:15pm**

Examining the evolution of oxygenic photosynthesis on the early Earth

Niki Parenteau[1], Linda L. Jahnke[1], Sherry Cady[2], and Beverly K. Pierson[3]

[1]NASA Ames Research Center, Mountain View, CA 94035
[2]Pacific Northwest National Lab, Richland, WA 99354
[3]University of Puget Sound, Tacoma, WA 98416

The evolution of the atmosphere, ocean, and microbial life on the early Earth were inextricably linked. The evolution of oxygenic photosynthesis and the resulting oxygenation of the atmosphere and oceans was arguably one of the most important events in the history of the young planet.

While modern cyanobacteria produce oxygen as a waste product from the oxidation of water, it may not have always been so. There is a large difference in the redox potentials between water used as an electron donor by cyanobacteria and hydrogen commonly used by the more ancient anoxygenic photosynthesis. Members of our group have speculated that an intermediate reductant such as Fe(II) could have bridged the gap and acted as a transitional electron donor before water. The widespread abundance of Fe(II) in Archean and Paleoproterozoic ferruginous oceans would have made it particularly suitable as an electron donor for photosynthesis. Therefore, iron-dependent photosynthesis using one photosystem in cyanobacteria may have been an important step in the evolution of oxygenic photosynthesis.

We have been searching for modern descendants of such an ancestral "missing link" cyanobacterium in a high-iron thermal springs. In our physiological ecology study of the cyanobacterial mats, we have found evidence that this type of metabolism is occurring *in situ* using carbon-14 bicarbonate uptake experiments and autoradiography. We have detected a stimulation of C-14 uptake in the presence of Fe(II) in lower light adapted cyanobacteria that inhabit the lower end of the photic zone in microbial mats. We are currently probing the metagenomic data obtained from the JGI Yellowstone National Park Community Sequencing Project for the molecular underpinnings of this process.

A complimentary study of the microbial biosignatures produced in these mats revealed diagnostic lipid biomarkers for cyanobacteria: mid-chain branched mono- and dimethylalkanes and, most notably, 2-methylhopanoids. This is the first documentation of 2-methylhopanoids in a modern iron-mineralized cyanobacterial mat where the cyanobacteria have been shown to grow anoxygenically using Fe(II) as an electron donor for photosynthesis.

The Mid-Infrared Imager/Spectrometer/Coronagraph Instrument (MISC) for the Origins Space Telescope

Thomas L. Roellig[1], Itsuki Sakon[2], Kimberly Ennico[1], and the MISC Instrument Study Team

1. NASA Ames Research Center, 2. The University of Tokyo

Abstract

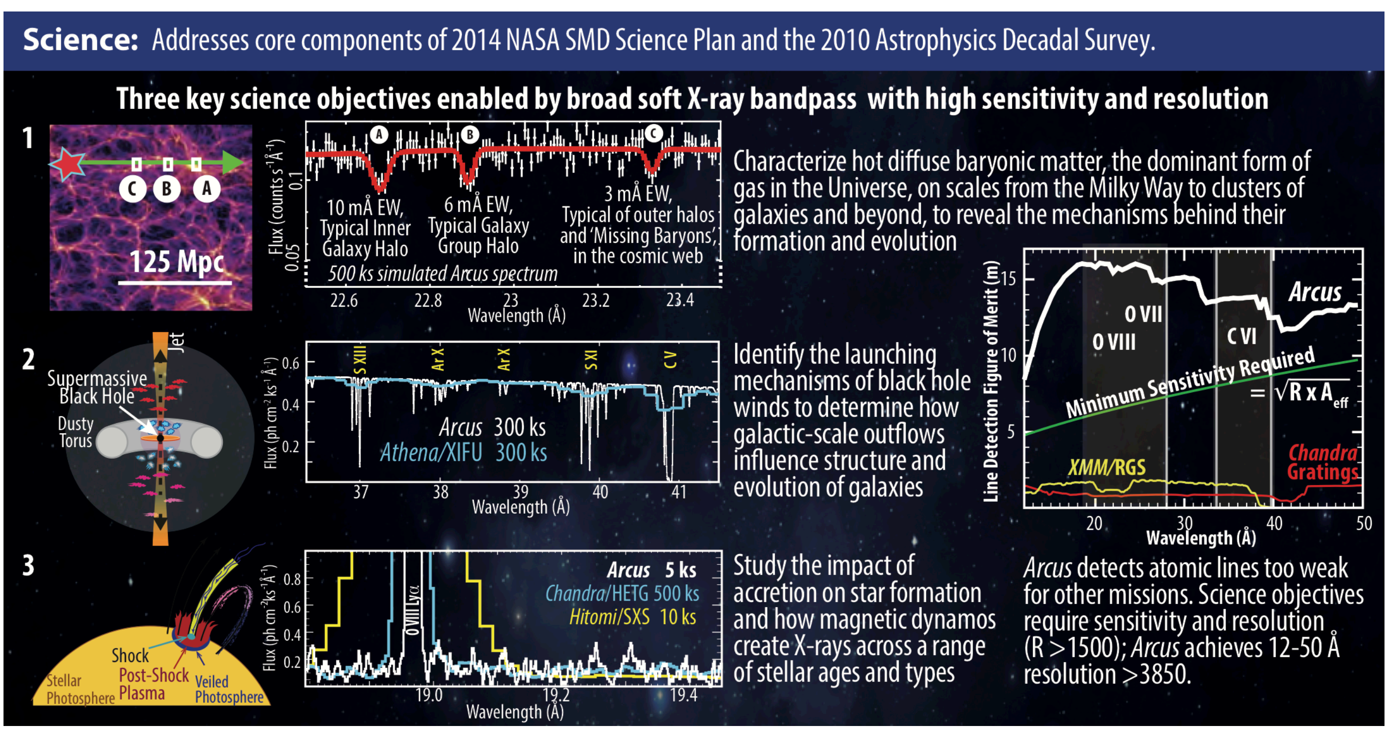
The Origins Space Telescope (OST) is one of four potential flagship missions that have been funded by NASA for study for consideration in the upcoming Astrophysics Decadal Review expected in 2020. The OST telescope will be up to 9.3 meters in diameter, cooled to ~4K, and the mission will be optimized for efficient mid and far-infrared astronomical observations. An initial suite of five focal plane instruments are being baselined for this observatory. The MISC instrument will observe at the shortest wavelengths of any of these instruments, ranging from 5 to 38 microns, and consists of three separate optical modules providing imaging, spectroscopy, and coronagraph capabilities. The imaging camera covers a 3' x 3' field with filters and grisms from 6-38 microns. The spectrometers have spectral resolving powers R~1,000 from 9-38 microns (with a goal of 5-38 microns) and R~25,000 for 12-18 and 25-36 microns. The coronagraph covers 6-38 microns. There is a special densified pupil spectrometer channel that would be used for R~100-300 exoplanet transit and emission spectroscopy from 6-26 microns with very high spectro-photometric stability. As the shortest wavelength focal plane imager the MISC instrument will also be used for focal plane guiding as needed for the other OST science instruments.

Oral Presentation: **3:40pm**

Title: *Arcus* - The X-ray Grating Spectrometer Explorer

Authors: Pasquale Temi (NASA – Ames) and the ARCUS Team

Arcus is a NASA/MIDEX Explorer mission that has been selected for Phase A study in August 2017. It is a free-flying satellite mission that will enable high-resolution soft X-ray spectroscopy (8-50Å) with unprecedented sensitivity – effective areas of >3500 sq cm and spectral resolution >2500. The Arcus key science goals are (1) to determine how baryons cycle in and out of galaxies by measuring the effects of structure formation imprinted upon the hot gas that is predicted to lie in extended halos around galaxies, groups, and clusters, (2) to determine how black holes influence their surroundings by tracing the propagation of out-flowing mass, energy and momentum from the vicinity of the black hole out to large scales and (3) to understand how accretion forms and evolves stars and circumstellar disks by observing hot infalling and out owing gas in these systems. *Arcus* relies upon grazing-incidence silicon pore X-ray optics with the same 12m focal length (achieved using an extendable optical bench) that will be used for the ESA Athena mission. The focused X-rays from these optics will then be diffracted by high-efficiency off-plane reflection gratings that have already been demonstrated on sub-orbital rocket flights, imaging the results with flight-proven CCD detectors and electronics. The power and telemetry requirements on the spacecraft are modest. The majority of mission operations will not be complex, as most observations will be long (~100 ksec), uninterrupted, and pre-planned, although there will be limited capabilities to observe targets of opportunity, such as tidal disruption events or supernovae with a 3-5 day turnaround. After the end of prime science, we plan to allow guest observations to maximize the science return to the community.



Ammonia on Charon: Laboratory Optical Constants of Ammonia Hydrates to Support *New Horizons* Observations

Authors: Joseph Roser[1,2], Alessandra Ricca[1,2], Cristina Dalle Ore[1,2], and Dale Cruikshank[2]
Affiliations: (1) SETI Institute (2) NASA-Ames Research Center

Abstract: An absorption feature at 2.21 μm has been detected on Pluto's moons Charon, Nix, and Hydra, as well as the dwarf planet Orcus and possibly Quaoar. This feature is believed to be indicative of ammonia and/or ammonia hydrates being present on the surface layers of these bodies. In the case of Charon, this is unusual since Charon's radiation environment is expected to destroy ammonia and ammonia hydrates rapidly. The discovery of these feature on the very small bodies Nix and Hydra and the discovery that ammonia on Charon is isolated within ammonia-rich, bright-rayed craters suggest that a sub-surface reservoir of ammonia, not cryovolcanism, may ultimately be responsible for this surface component. In this view, the ammonia molecules in the shallow interior diffuse through the water ice that covers the satellite, acquiring a hydrate structure as it reaches the exposed surface. This can be seen as a continuing process as NH_3 is destroyed when exposed to solar ultraviolet light and is then replenished as more ammonia diffuses upward. Published laboratory studies support the conversion of NH_3 to $NH_3{\cdot}nH_2O$ as it diffuses through pure H_2O ice.

To better understand the origin of this 2.21 μm feature, we have undertaken a combined program of laboratory experiments to be conducted at NASA-Ames Research Center to measure the optical constants of ammonia/water ice mixtures and ammonia hydrates in addition to quantum chemistry calculations for these systems. These data will be used in models of Charon's reflectance spectrum in order to better determine the specific ammonia ices present on Charon.

Pollack Lecture: **4:20pm**
Linda Jahnke

Biosignatures for life detection.

Linda L. Jahnke

Abstract:
Life on Earth arose more than 3 billion years ago on the surface of a planetary body very different than today, one which would have seemed inhospitable to most modern organisms. The first 'living' cells survived and evolved in response to many physical challenges, and ultimately left the signatures of this evolutionary heritage in the geological record. For years, we have studied modern microorganisms and their natural environments for clues, the 'biosignatures', that establish connections between major evolutionary events and their geological consequences to Earth's planetary evolution. These biosignatures are 'fossil' characteristics of cells that leave a preserved record but they are the products of fundamental microbial physiology. Together they form the basis of our knowledge for 'Life Detection'. Our understanding of modern biology has expanded our view of the diversity, metabolic versatility and tenacity of microbial life on Earth. Now, we seek to apply this understanding to the detection of signatures for Life beyond their planet of origin to other worlds.

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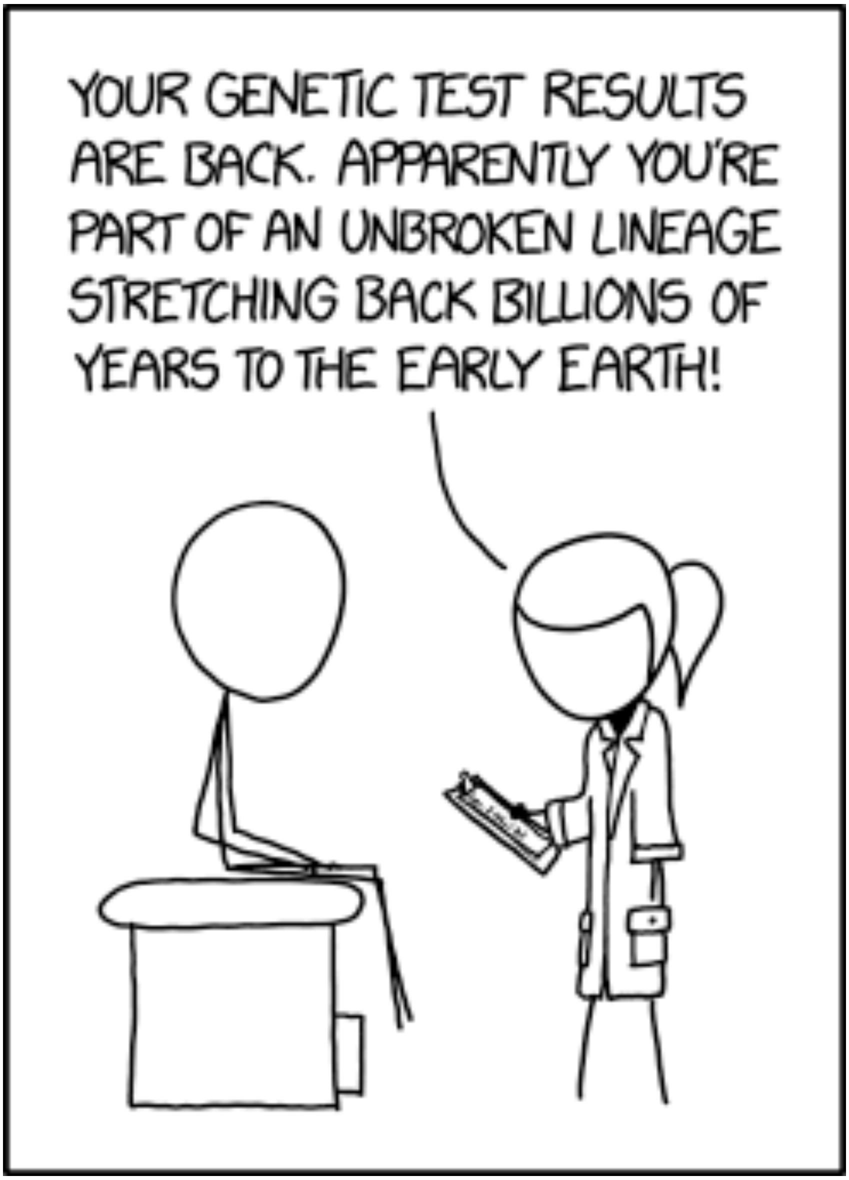

https://xkcd.com/1840/

Astrobiology Poster: **AB.1**

Enceladus Life Signs And Habitability (ELSAH) mission

Chris McKay, Alfonso Davila, Jen Heldmann, Richard Quinn, Tori Hoehler, Niki Parenteau, Tony Ricco, Carol Stoker, David Willson (The members of the ELSAH Development Team at NASA Ames).

ELSAH is a mission to explore and sample the plume of material emerging from Enceladus' South Polar Terrain. Its science goals are to search for biosignatures in the plume, assess the habitability of Enceladus' subsurface ocean, and to examine the plume's overall structure and dynamics. The goals of identifying biosignatures and assessing habitability will be addressed using two in-situ instruments: a mass spectrometer called PALMS and a wet chemistry lab system called μCAFÉ. These instruments will receive particle and gaseous material from the plume and examine various chemical indicators of habitable environments and life, including redox state, distributions and chirality of amino acids, and distributions of fatty acids. These instruments will sample the plume over a series of flybys where the spacecraft flies through the base of the plume at low (<1.5 km/s) encounter speeds. The goal of characterizing the moon's overall activity will be addressed by two remote-sensing instruments, a visible camera called NAC and a thermal infrared instrument called ENTIR. NAC will observe the plume prior to the first close encounter in order to characterize Enceladus' activity, while both ENTIR and NAC will map the South Polar Terrain during each flyby to identify sources and characterize their geological context.

ABIOTIC SYNTHESIS OF NUCLEOBASES IN ASTROPHYSICALLY RELEVANT ICES.

C. K. Materese[1,2], M. Nuevo[1,2], P.P. Bera[1,2], T.J. Lee[1] and S. A. Sandford[1], [1]NASA Ames Research Center, Moffett Field, CA, USA, [2]BAER Institute, Moffett Field, CA, USA

Introduction: Nucleobases are biomolecules that act as the fundamental components of the alphabet from which known life is encoded (Fig. 1). They are highly conserved between species and were likely important during the early emergence of life. To date, no experimental conditions have been determined that could abiotically produce all of the primary biological nucleobases in a terrestrial environment or in an early terrestrial analog.

We have demonstrated, experimentally and computationally, that it is possible to produce all of the biological nucleobases from the UV-irradiation of pyrimidine and purine in simple astrophysical ice analogs [1-7]. Here we present a full summary of the results of all of our efforts on this topic.

Experimental: Volatile gases were premixed in ~2L bulbs which were attached to a cryogenic vacuum chamber. Purine was prepared separately in an evacuated sample tube that was attached directly to the vacuum chamber, and wrapped with heat tape and a thermocouple to control and monitor the temperature and deposition rate. Reactants were vapor deposited onto a cooled substrate in the vacuum chamber that maintained a temperature of ~15K. Throughout deposition, the ice were simultaneously irradiated with an H_2-discharge lamp emitting UV photons (Lyman α at 121.6 nm and a continuum centered at ~160 nm). After irradiation, samples were warmed to room temperature, and refractory residues were recovered for derivatization and analysis.

Computational: Structures and energies of the reactants, intermediates, and products along the reaction path were calculated using modern range-separated hybrid meta-GGA (wB97M-V) density functional methods (DFT) along with large basis sets for both gas phase as well as condensed phase conditions. The effects of the extended ice environment were modeled by a conductor-like polarized continuum model (C-PCM) in which the bulk is represented as a polizable medium characterized by its dielectric constant.

Results: Our work has demonstrated that the UV-photoirradiation of pyrimidine and purine in astrophypsical ice analogs leads to the production of all of the primary nucleobases, and numerous other compounds of potential prebiotic interest. The relative abundances of these compounds is heavily dependent on the following: 1) The composition of the starting ice mixture, which impacts the type of functional groups available for substitution, the proton affinity of the surroundings, the UV-cross section, and the number of species in competition for substitution; 2) the number of functional group additions required to form the product. More substitutions requires more photons and more potential ways for the production pathway to be disrupted; 3) The type of functional group added to pyrimidine or purine. Functional groups are produced with different efficiencies from the reactant ices and the energetic favorability of their additions to pyrimidine or purine plays a role; 4) The position where the addition takes place is also important for both energetic (e.g. ease of deprotonation) and statistical reasons (e.g. numerous ways to produce identical isomers).

The ice matrix plays very important, and sometimes contradictory, roles as a medium for reaction, and as a progenitor of ions. The mechanisms involving a cationic route dominate. The gas phase mechanism of formation of nucleobasee is ineffective, and the presence of condensed phase is necessary.

Conclusion: Our results demonstrate that all biological nucleobases can be produced under similar astrophysical conditions. These nucleobases and other pyrimidine and purine derivatives are produced with large differences in their relative abundances. If compounds of astrophysical origin are important for the emergence of life, our results suggest that some nucleobases (uracil, cytosine, and adenine) were far more abundant than others (thymine and guanine) and may suggest that some alternative compounds (e.g. hypoxanthine, a guanine substitute) may have played roles early in the evolution of life.

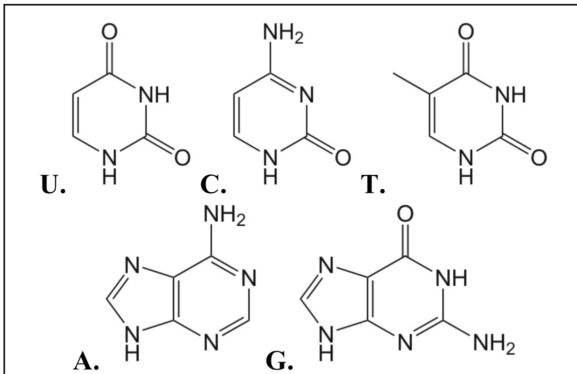

Fig. 1. The five primary biological nucleobases. **U.** Uracil **C.** Cytosine **T.** Thymine **A.** Adenine **G.** Guanine

References: [1] Nuevo M. et al. (2009) *Astrobiology,* 9, 683. [2] Bera P. P. et al. (2010) *JCP*, 133, 104303 [3] Nuevo M. et al. (2012) *Astrobiology,* 12, 295. [4] Materese C. K. et al. (2013) *Astrobiology,* 13, 948. [5] Nuevo M. et al. (2014) *ApJ*, 793, 125. Bera P. P. et al. (2016) *JCP,* 144, 144308. [6] Materese C. K. et al. (2017) *Astrobiology,* 17, 761. [7] Bera P. P. et al. (2017) *Astrobiology,* 17, 771.

An Inventory of the Sugar Derivatives in Residues Produced from the UV Irradiation of Astrophysical Ice Analogs

Michel Nuevo,[1,2,*] George W. Cooper,[1] John M. Saunders,[3] Christina E. Buffo,[4] Christopher K. Materese,[1,2] and Scott A. Sandford[1]
[1]*NASA Ames*; [2]*BAER Institute*; [3]*UC Santa Cruz*; [4]*Wellesley College*
*e-mail: michel.nuevo-1@nasa.gov

Carbonaceous meteorites such as Murchison and Murray contain a large variety of organics of astrobiological interest such as amino acids, functionalized polycylic aromatic hydrocarbons (including quinones), functionalized nitrogen heterocycles (including nucleobases), amphiphilic compounds (whose structure has yet to be determined), and sugar derivatives. The presence of such a broad variety of meteoritic organics strongly suggests that molecules important for life can form abiotically under astrophysical conditions. This hypothesis is supported by laboratory work in which mixtures of astrophysical ice analogs (H_2O, CO, CO_2, CH_3OH, CH_4, NH_3, etc.) are exposed to ultraviolet (UV) irradiation at low temperature (<15 K) to simulate cold interstellar and protoplanetary environments. These experiments have shown that the organic materials (residues) recovered at room temperature contain organics that are similar to those found in meteorites.

However, no systematic search for the presence of sugar derivatives in such residues had been carried out until recently, with the detection of ribose as well as other sugars and sugar derivatives in one residue produced from the UV irradiation of an H_2O:CH_3OH:NH_3 ice mixture at 80 K. In this work, we performed several experiments in which ice mixtures containing H_2O, CH_3OH, CO, CO_2, and/or NH_3 were UV irradiated at 10 K, and carried out a systematic search for sugars and sugar derivatives. Results confirm the presence of a wide variety of sugar alcohols, sugars, and sugar acids with up to 6 carbon atoms, including ribose, and show the presence of several other variants of sugar derivatives. The distribution of the sugar derivatives found in our residues constrains their formation in these experiments. Finally, our experimental results are compared with meteoritic data.

Development of microbial production platforms for high-strength polymers for space and earth applications

Nils JH Averesch[1,3], Jens O Krömer[2,3], Lynn J Rothschild[4]

[1] Universities Space Research Association at NASA Ames Research Center, Moffett Field, CA, USA
[2] Department of Solar Materials, Helmholtz Centre of Environmental Research - UFZ, Leipzig, Germany
[3] The University of Queensland, Advanced Water Management Center, Brisbane, Australia
[4] Planetary Systems Branch, NASA Ames Research Center, Moffett Field, CA, USA

Plastics and (high strength) polymers are not only omnipresent in everyday life, but of particular importance in space technology. Polyethylene terephthalate (PET) is the most common thermoplastic polyester, with a wealth of applications from commodities like synthetic fibers for clothing and blow molding of bottles to speciality applications: Biaxially-oriented polyethylene terephthalate (BoPET, trade name Mylar®) is valued for its high tensile strength, chemical and dimensional stability, barrier properties and electrical insulation; layers of metallised BoPET are for example used in NASA's spacesuits for thermal insulation and radiation resistance. The thermoplastic Vectran™ is another aromatic polyester-fiber with outstanding tensile properties, including high tenacity and high strength modulus. The toughness and rigidity of Vectran™, while weighing in low, led to its use in NASA's Pathfinder, Spirit and Opportunity Mars landers. Aramids, like the fabric and sheet material Kevlar®, feature similarly outstanding fiber tensile properties, as well as excellent chemical- and thermal-stability as well as radiation resistance. They are indispensable for a range of speciality applications like ballistic protection. Therefore, these materials are especially suited for space technology in construction of environmental suits and habitations, as the use in Bigelow Aerospace's inflatable spacecrafts shows.

The feedstocks of these materials are commonly fossil-fuel derived, which is neither sustainable in the long run on Earth, nor available in space or at destinations such as Earth's moon or Mars. Metabolic Engineering may solve these problems, by enabling production of bio-replacement precursors, and potentially also by realising bio-based production of novel aramid-fibers. The core compounds are the aromatics *para*-hydroxybenzoic acid and *para*-aminobenzoic acid (pHBA & pABA). The former is a major feedstock for production of liquid crystal polymers; most importantly it is one of the two monomers of the poly-condensate Vectran™. The latter may be polymerized to form a material with a molecular structure analogous to Kevlar®, or can be converted to terephthalic acid as feedstock for production of PET / Mylar®. Using an approach that combines metabolic modelling with genetic engineering, microbial production systems for pHBA and pABA have successfully been established.

For pHBA, a *Saccharomyces cerevisiae* based microbial production system was developed, which delivered a final titer of 2.9 g/L, a peak specific rate of 18.6 mg/(g_{CDW}×h), carbon-yields of up to 4.7% [C-mol/C-mol] (3.1 $mg_{pHBA}/g_{glucose}$) and a productivity of 27.4 mg/h in a fed-batch bioreactor process. For production of pABA, the previously developed *S. cerevisiae* based microbial cell factory was translated for application in *Bacillus subtilis*, the organism of choice in space synthetic biology. Production of pABA in *B. subtilis* reached titers of 3.22 g/L, carbon-yields of over 12% [C-mol/C-mol] (corresponds to 16.5% of the theoretical maximum) and rates of 50 mg/h. The highest production was achieved on an amino-sugar based carbon-source, proving the suitability of the system for *in situ* resource utilization, when utilising feedstocks such as cyanobacterial cell lysate in space biotechnology.

Engaging the Public with MarsFest Events in Death Valley National Park. R. Bonaccorsi[1,2,], C.P. McKay[2], D. Willson[2], A.P. Zent[2], A. Davila[2], C.R. Stoker[2], D. Blaker[3] D. Scalice[2], E. DeVore[1], [1]SETI Institute (Mountain View, CA 94043) (rosalba.bonaccorsi-1@nasa.gov) [2]NASA Ames Research Center (Moffett Field CA 94035); Death Valley Natural History AssociatioDeath Valley, CA 92328

One of NASA's key programs is the exploration of Mars. Since the late 1980's Mars-like deserts on Earth such as Death Valley have been used to better understand their morphological and environmental counterparts observed of our Solar System's planetary bodies and to prepare for Mars missions.

Over the past seven years (2011-2018) we have worked together to organize MarsFest events in Death Valley National Park (DVNP). The goal of MarsFest is to elevate public awareness about planetary analog research here on Earth, and the associated NASA missions in space, such as the Mars Science Laboratory (MSL) and 2020 rovers [1-2]. The event was so successful and well received by the participating scientists, the Park Rangers, and the general public that has become an annual event. A MarsFest event is again being organized for February 24-25, 2018.

MarsFest public outreach activity is an important part of communicating about NASA missions and showing the connection to life on Earth. Events such MarsFest foster the cooperative effort between NASA and the National Park Service (NPS) and enhance the interpretive rangers' understanding of the NASA research. MarsFest key sponsors and partners are from the SETI Institute, Death Valley Natural History Association, Death Valley National Park, NASA Ames Research Center (ARC), NASA Goddard Space Flight Center (GSFC) Sample Analysis at Mars (SAM), JPL (Jet Propulsion Laboratory), and the Mars Society. Over the years, the NASA ARC's Public Engagement office produced clips for NASA TV and the NASA Ames YouTube Channel [2]. Copies of the last years Astrobiology Jamboree proceedings were displayed at the NASA Ames/ SETI Institute-staffed booths. In 2017 the activities drew in over 2,500 visitors over the first 2 days.

Event description and outcomes: A typical 3-day event features *i)* evening keynote speakers and panels, *ii)* field trips to analog sites co-led by NPS and planetary scientists, *iii)* an exposition with hand-on activities (Figures 1-2), and *iv)* night sky viewing events. These activities are designed for visitors of all ages and interest levels and run throughout the day from Friday through Sunday. As an example, in 2016 NASA Ames scientists Carol Stoker and David Willson gave demonstrations of the Mars Icebreaker payload (Figure 1). In the evening, Margaret Race, Alfonso Davila (NASA Ames), and Brian Day (NASA SSERVI) contributed to a panel on the protection of National Parks, analog sites, and other celestial bodies during robotic and human exploration. After the panel, C. McKay (ARC) gave a highlight presentation about the search for life on Ocean Worlds [3]. Field trips have been led to Badwater's microbial-rich evaporite deposits (S. Douglas), and the Mars-like Mars Hill and Mesquite Flat Sand Dunes (Aaron Zent, ARC). The former location is geomorphologically similar to the Viking 1 and Pathfinder landing sites. R. Bonaccorsi (SETI Institute at ARC) and B. Haberle (ARC) guided visitors through the Ubehebe Volcanic Field, a proposed analog test site for claystone deposits investigated by Curiosity [e.g.,4]. Over 45 volunteers from the Bay Area and Southern California helped operate booths and lead public events. Support for the festival comes from several senior and junior scientists, students, education and outreach professionals, astronomy club members, and planetary science enthusiasts (e.g., The Mars Society, Planetary Society) who volunteer to share their time, resources, and knowledge with Park's visitors. In 2016 some financial aid was provided by the NASA Astrobiology Institute.

Figure 1. Demonstration of Icebreaker Lander.

Figure 2. Alfonso Davila talking science with visitors.

References: [1] http://www.seti.org/marsfest2013; [2] https://www.youtube.com/watch?v=Csfg_noH-l4 [3] http://www.seti.org/celestial_centennial_marsfest_2016; [4] Grotzinger et al. 2012, *Space Sci. Rev., 170,* 5–56.

Stanford-Brown iGEM 2017: Mars: Getting there and staying there

Stanford University: Marilus Bravo, Addie Peterson, Michael Herschl, Katie Guy, Natalie Baker (students) **Kara Rogers** (staff)

Brown University: Nischal Acharya, Ileana Pirozzi, Emmett Askira, Dylan Spangle, Sierra Harken, Brian Vuong (students) **James Head, Gary Wessel** (faculty)

NASA ARC: **Lynn J. Rothschild** (cs), Trevor! Kalkus, Kosuke Fujishima, Gordon Sun, Nils Averesch (USRA)

ASTROBIOLOGY

The iGEM (international Genetically Engineer Machine) competition requires teams to create DNA constructs that can contribute to research and the bioengineering toolbox. Since 2011, the Rothschild Lab has hosted students from Stanford and Brown University for the iGEM competition, adding Spelman in 2014. Projects have included a synbio-based Mars colony, synthetic astrobiology, a biodegradable drone, self-folding origami and a bioballoon. Biological materials have advantages over traditional building materials; most significantly, they are cheap, light, and self-replicating. These characteristics make biomaterials ideally suited for space exploration.

The 2017 Stanford-Brown team assessed the advantages of biological solutions to space exploration, namely the self-sustaining abilities of low-mass organisms to make planetary more self-sufficient and economical paper (http://2017.igem.org/Team:Stanford-Brown). Prioritizing repair over replacement, the team developed self-healing materials embedded with *Bacillus subtilis*. For longer-lasting energy, they designed a "biobactery" using linearly oriented *E. coli* to generate power. For renewable materials, they engineered bacteria to synthesize and degrade rubber. Individually these projects offer sustainable alternatives for repair, power and materials. When combined, these insights can provide us with the power to get to Mars and the resources to sustain us while we are there.

In addition to the lab-based synthetic biology and materials testing research, the team conducted outreach at the Bay Area and New York Maker Faires. They investigated the economics of producing rubber with microbes, visiting and interviewing Dupont and Amyris, and the USDA resulting in a white paper (http://2017.igem.org/Team:Stanford-Brown/HP/Gold_Integrated). They had the opportunity to discuss the use of synthetic biology in space exploration with Dr. Pascale Ehrenfreund, Chair of the DLR Executive Board. Particularly exciting was the selection by NOVA to film the team and interview them on their work. The show is anticipated to air during the summer of 2018.

Constraints on the Metabolic Activity of Microorganisms in Atacama Surface Soils Inferred from Refractory Biomarkers: Implications for Martian Habitability and Biomarker Detection.

Mary Beth Wilhelm[1,2], Alfonso F. Davila[1], Mary N. Parenteau[1], Linda L. Jahnke[1], Mastewal Abate[1], George Cooper[1], E. Taylor Kelly[3], Victor Parro García[4], Miriam G. Villadangos[4], Yolanda Blanco [4], Brian Glass[5], James J. Wray[2], Jennifer L. Eigenbrode[6], Roger E. Summons[7], Kimberly Warren-Rhodes[3]

[1]Space Science and Astrobiology Division, NASA Ames Research Center; [2]School of Earth and Atmospheric Sciences, Georgia Institute of Technology; [3]Carl Sagan Center, SETI Institute; [4]Departamento Evolución Molecular, Centro de Astrobiologia (INTA-CSIC), Madrid, Spain; [5]Intelligent Systems Division, NASA Ames; [6]Planetary Environments Laboratory, NASA Goddard; [7]Department of Earth, Atmospheric, and Planetary Sciences, Massachusetts Institute of Technology

Abstract: Dryness is one of the main environmental challenges to microbial survival. Understanding the threshold of microbial tolerance to extreme dryness is relevant to better constrain the environmental limits of life on Earth, and also to critically evaluate long-term habitability models of Mars. Biomolecular proxies for microbial adaptation and growth were measured in Mars-like hyperarid surface soils in the Atacama Desert that experience only few millimeters of precipitation per decade, and in biologically active soils a few hundred kilometers away that experience 2-5 fold more precipitation. Diversity and abundance of lipids and other biomolecules decreased with increasing dryness. Cyclopropane fatty acids (CFA), indicative of adaptive response to environmental stress and growth in bacteria, were only detected in the wetter surface soils. The ratio of *trans* to *cis* isomers of an unsaturated fatty acid, another bacterial stress indicator, decreased with increasingly dry conditions. Aspartic acid racemization ratios increased from 0.01 in the wetter soils to 0.1 in the driest soils, indicative of racemization rates comparable to *de novo* biosynthesis over long time scales (~10,000 years). The content and integrity of stress proteins profiled by immunoassays were additional indicators that biomass in the driest soils is not recycled at significant levels. Together, our results point to minimal or no *in situ* microbial growth in the driest surface soils of the Atacama, and any metabolic activity is likely to be basal, for cellular repair and maintenance only. Our data add to a growing body of evidence that the driest Atacama surface soils represent a threshold for long-term habitability (i.e., growth and reproduction). These results place constraints on the potential for extant life on the surface of Mars, which is 100-1000 times drier than the driest regions in the Atacama.

Testing Ice Collection For Europa & Enceladus Plume Fly-Through Missions.

D. Willson[1], R. Bonaccorsi[1,3], R. Gold[2], E. Adams[2], S. Thomson[1] , D. Slone[4], D. Mathias[1], J. Koehne[1] & C.P. McKay[1]
[1] NASA Ames Research Center, M.S. 245-3, Moffett field, 94035 CA, david.willson@nasa.gov ,
[2]Applied Physics Laboratory, The Johns Hopkins University, 11100 Johns Hopkins Road, Laurel MD 20723,
[3]Carl Sagan Center at the SETI Institute. 189 Bernardo Ave., Suite 100. Mountain View, CA 94043-5203.
[4] Whitman Collage 345 Boyer Ave Walla Walla WA,

Science Topic: Astrobiology, Presentation & Poster

Introduction: The plumes at Europa and Enceladus provide an opportunity to determine their habitability and presence of life signatures by collecting the plume ice particles. The Cassini spacecraft has flown through the Enceladus geyser plumes at speeds >7 km/sec [1] with a Cosmic Dust Analyser [2] and an Ion Neutral Mass Spectrometer [3] and measured spectra of plasma generated by impacting plume ice particles. These measurements were limited by the high flythrough speeds, as large organics impacting the instruments were destroyed or altered [4]. Flying through the plumes at slower speeds allows for collecting ice particles in pristine condition where microbes or large biomolecules are intact for analysis. The Johns Hopkins University Applied Physics Laboratory (JUH/APL) and NASA Ames Research Center (ARC) are conducting tests to collect simulated ice plume at slower fly-throughs speeds using the ARC Vertical Gun (Fig. 1).

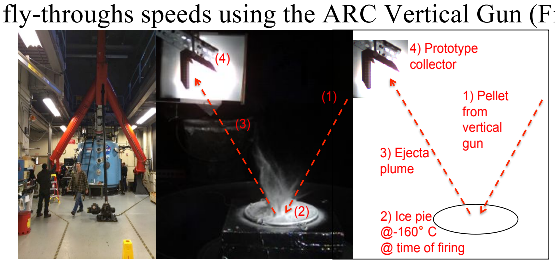

Figure 1: (Left) ARC Vertical Gun. (Middle & Right) Prototype collector & ice pie setup.

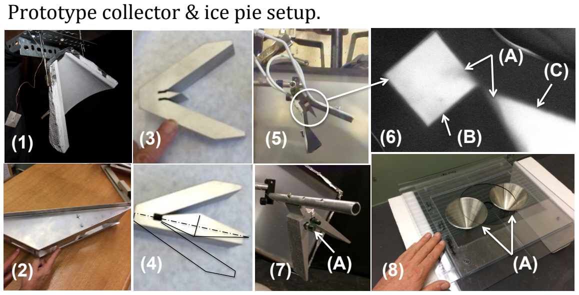

Figure 2: (1) & (2) Early collectors, (3) & (4) Various cross-sections tested, (5) LN_2 cooled collector for ice particle speed & size test, (6) (A) Incoming ice particles, (B) collection chamber & (C) Collector funnel wall, (7) LN_2 cooled Collector with (A) removable collection tubes for organics testing, (8) Efficiency test collectors using 3-8µm Poly Methyl Methacrylate (PMMA) spheres.

Methods: (1) *Apparatus:* Plumes of 140° K ice particles travelling up to 2.3 km/s were created by shooting 3-mm hollow aluminium pellets (up to 6 km/s) at liquid-nitrogen-cooled ice cakes of Natural Seawater (NS), Synthetic Seawater (SSW), and Distilled Water (DW) blanks as controls. Funnel collectors were positioned to test ice particle capture (Fig. 2) and their impact speeds were measured and filmed at resolutions of 50 µm. Smashing upon impact, the fragments are funnelled into a collection chamber (Fig. 2-6). PMMA micro-spheres were shot into the collector to test its efficiency (Fig 2-8).

***(2)** Organics Survival Upon Impact:*

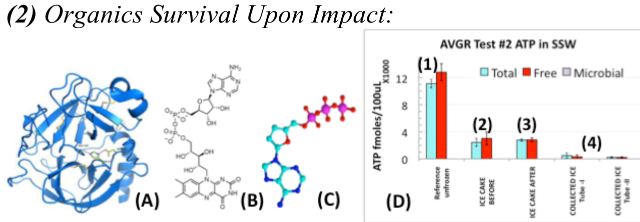

Figure 3: (A) Trypsin, (B) Flavin Adenine Dinucleotide (FAD) & (C) Adenosin Triphosphate (ATP), (D) Table of : Total, Free & Microbial ATP concentrations in synthetic sea water (1), Ice before (2) & after (3) shoot & at collection (4).

Microbial and free ATP, Trypsin, FAD, and amino acid Lysine were used as proxy for microbial survival as well as for biomarker impact survival tests (Fig. 3). Organics concentrations were measured in: (1) sea water before freezing, (2) ice cakes before and (3) after pellet firing, and (4) melted or sublimated ice in collectors. NASA Planetary Protection practices [5] applied cleaning protocols for microbial reduction in the shooting chamber, and bioburden monitoring using an ultrasensitive ATP luminometry assay (LOD: 0.2×10^{-15} moles (femtomoles), for prescreening of collectors surfaces, which is below the threshold cleanliness limit of 2.3×10^{-11} mmol ATP/ 25 cm^2 (0.9 $fmoles/cm^2$) [6].

***(3)** Computer simulation modelling:* Simulated impacts of ice particles on an aluminium surface at 30° were modeled, at 1500 m/sec, using ALE3D hydrocode from LLNL. Modelling involved a simple equation of state using bulk modulus and stress/strain based failure criteria (Fig. 4). The modeling has assisted in finding collection efficiency and affirming organics survival.

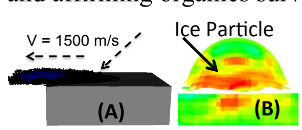

Figure 4: (A) Simulation of a 1.5 km/sec impact on Aluminum showing fragmentation. (B) Pressure stress in ice particle at 1.5 km/sec impact affirming amino acid survival.

Conclusion: The Vertical Gun and computer simulation results show particles smash upon impact at ~1.5 km/sec and flow into the sample chamber with >90% efficiency (the efficiency tests are still ongoing). Organic biomarker survival upon impact is significant for Trypsin, FAD and Lysine; the fragile free ATP molecule in SSW and microbes in natural seawater have low survival.

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NEW DEVELOPMENTS IN X-RAY DIFFRACTION FOR PLANETARY EXPLORATION.
D. Blake[1], P. Sarrazin[2], M. Gailhanou[3], J. Chen[4], P. Dera[5], B. Downs[6], R. Walroth[1] and T. Bristow[1], [1] Exobiology Branch, NASA Ames Research Center, Moffett Field, CA 94035, [2] SETI Institute, Mountain View, CA 94043, [3] CNRS, IM2NP UMR, Marseille, France, [4] Baja Technology, Tempe, AZ, [5] HIGP, Univ. of Hawaiʻi, Honolulu, HI, [6] Geosciences, Univ. Arizona, Tucson AZ 85721-0077.

Introduction: X-ray diffraction (XRD) is the gold standard for definitive, quantitative mineralogical analysis. The MSL CheMin instrument established the quantitative mineralogy of the Mars soil [1], characterized the first habitable environment on another planet [2], and provided the first *in-situ* evidence of Martian silicic volcanism [3]. CheMin is now characterizing lacustrine mudstones that comprise the lower strata of Mt. Sharp [4] that contain evidence of the gradual dessication and oxidation of the Mars surface.

Even with its simplified sample movement system, CheMin still requires substantial sample preparation. Deployment of XRDs on smaller missions will require simplified sample preparation, decreased instrument size and complexity, and improved 2θ resolution. Efforts in these directions are underway.

XRD with Limited Sample Preparation: XTRA (Extraterrestrial Regolith Analyzer) will analyze fines in as-delivered surface regolith [5]. Fine-grained regolith coats the surfaces of most airless bodies in the solar system, and can often be used as a proxy for the surface mineralogy. XTRA can be configured in transmission or reflection geometry using vibrated cells for as-delivered powders, allowing direct analysis of materials scooped at the surface.

XRD without Sample Preparation: Hybrid-XRD (HXRD) is concept under development to analyze rocks or soils without sample preparation [6]. If the material is sufficiently fine-grained, a powder XRD pattern is obtained, similar to CheMin or XTRA. With coarse-grained crystals, the white bremsstrahlung radiation of the tube is diffracted into single crystal Laue patterns. Unlike typical Laue applications, HXRD analyzes the energy of each Laue spot, enabling the measurement of single crystal Bragg diffractions. Dedicated crystallographic software has been developed for identification of minerals responsible for the Laue patterns.

High resolution XRD: With CheMin and any of the previously described XRD concepts, instrument resolution suffers from system miniaturization and is limited to about 0.3°2θ. A planetary XRD based on Guinier geometry is under development to provide a compact high-resolution instrument. A substantial gain in resolution has been demonstrated with a basic proof-of-concept instrument. Both reflection and transmission geometries can be developed with the Guinier design and are being explored as part of a PICASSO funded project.

Development of High TRL Components: High TRL subsystems are being developed for future XRD instruments. Special CCD detectors are being developed with e2V (UK (Fig. 1A). Custom FPGA based electronics for low noise CCD operation with embedded data processing capabilities are under development with Baja Technology (Fig. 1B). Miniature X-ray tubes are being developed in collaboration with RTW of Germany (Fig. 1C) that are compatible with power supplies developed by Battel Engineering (Fig. 1D).

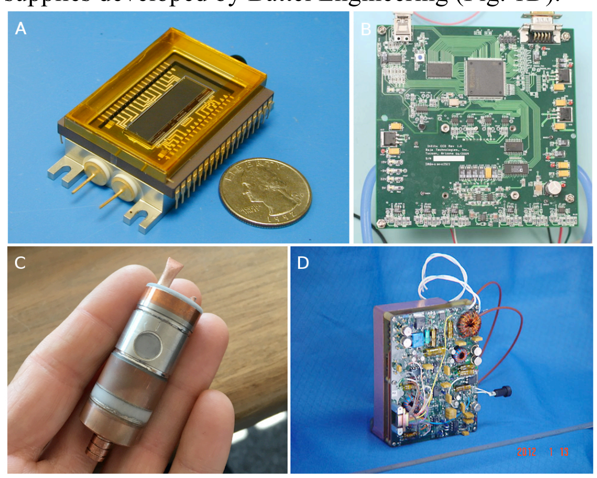

Fig 1: Example of flight components under development with industrial partners: A. X-ray CCD in flight package with internal peltier cooler (e2V); B. CCD control electronics (Baja Technologies); C. Miniature microfocused X-ray tube (RTW); D. X-ray tube power module with HVPS stage (Battel Engineering).

Deployment Opportunities: Future instruments proposed for flight will be tailored to the specific mission constraints and will be comprised of combinations of the features and flight hardware presented above.

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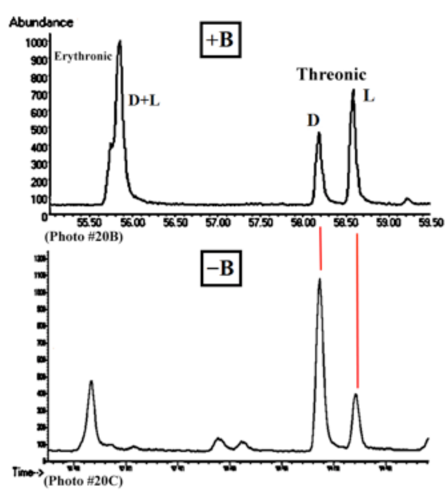
Enantiomer Excesses In Meteoritic Organic Compounds: A Role For Radiation-Magnetism? G. Cooper and A. C. Rios - Exobiology Branch, george.cooper@nasa.gov, andro.c.rios@nasa.gov

Carbonaceous chondrites contain an insoluble “macromolecular” carbon phase as well as discrete soluble organic compounds including amino acids and sugar derivatives. Both the macromolecular carbon and the sugar derivatives are thought to have formed through extraterrestrial aqueous formaldehyde chemistry. Our project involves the utilization of formaldehyde reactions to produce chiral compounds, i.e., compounds that are composed of two non-superposable mirror images or "enantiomers", analogous to a left and right hand. Such molecules are important in con-temporary life because biological polymers (proteins, nucleic acids, etc.) are homochiral, i.e., their monomers consist of only one of the two enantiomers. In contrast, it has been shown, at least in one lab setting, that abiotic syntheses of significantly sized RNA polymers do not proceed if the monomers are present in racemic (50:50) mixtures due to "enantiomeric cross-inhibition". In general, there is a scarcity of prebiotically plausible mechanisms that are capable of inducing enantiomer excesses. Therefore, there is a need to uncover plausible abiotic mechanisms (if any) that could have led to net enantiomer enrichments. Two laboratory accessible mechanisms have stood out for creating actual net enantiomer excesses in organic compounds: (1) the slight preferential destruction of one enantiomer by circularly polarized UV light. At low temperatures such methods might also synthesize compounds containing enantiomer excesses and (2) photo-magnetic effects: so far applied only to pre-made inorganic (metal) complexes. In the latter case, although the resulting enantiomer excesses are very small (~ 10^{-4}), the authors demonstrate reversible excesses with opposite magnetic direction. Powerful magnetic fields (up to ~ 15T) were required. We are also attempting to synthesize compounds under the influence of magnetic fields and radiation. However, in contrast to the above photo-magnetic experiments, we are attempting to create enantiomer excesses (1) during the actual synthesis of the target compounds (2) in prebiotically plausible and relevant compounds (sugars and their derivatives) and (3) under much milder prebiotic conditions. This work may determine if the early interaction between organic precursor compounds and radiation and magnetism could have led to (at least) a portion of the enantiomer excesses observed in carbonaceous chondrites.

Reaction mixtures are typically placed in magnetic and photo fields of varying strengths. Mixtures consist of formaldehyde and salts known to be present in carbonaceous chondrites (Ca^{2+}, Na^{+}, SO_4^{2-}, CO_3^{2-}, etc.): most analyses are by gas chromatography-mass spectrometry (GC-MS) and liquid chromatography-mass spectrometry (LC-MS).

Figure 1 shows the result of just one preliminary experiment aimed at the creation of reversible photo-magnetic enantiomer excess. This and other aspects and results of experiments will be presented.

Figure 1. Results of one photo-formose experiment showing the apparent creation of reversible enantiomer excesses. +B and –B refer to opposite magnet-ic field direction: otherwise, the two runs were per-formed under nearly identical conditions. Several other compounds (not shown) are also present.



An Astrobiology Outreach Activity: Meteorites, Organic molecules and the Origin of Life

Andro C. Rios[1] and George Cooper[2], [1]Blue Marble Space Institute of Science. [2] Exobiology Branch, NASA Ames Research Center, Andro.c.rios@nasa.gov.

Carbonaceous chondrites are important to the field of astrobiology because the molecules they contain provide a record to the organic chemistry that took place in the early Solar System before the emergence of life on Earth. These meteorites also provide an opportunity to introduce general organic chemistry concepts that are relevant to astrobiology for public outreach events. We have built upon our previously reported classroom activity (1) to tailor an engaging and tangible structure-smell relationship for participants as they learn about the chemical classes of molecules found in meteorites. The outreach activity can be truncated or expanded in its science content depending on the age distribution of participants and venue type, such as large public science expos or intimate seminar/classroom settings. After being introduced to some of the typical broad questions associated with astrobiology. i.e., How did life start on Earth? Does life exist elsewhere? Participants are introduced to how meteorites are uniquely suited to helping astrobiologists address aspects of these questions. We often include a meteorite on display with some additional instructional aids at these events as well. Participants then use their noses to explore the odor differences of organic molecules that represent classes of organic compounds found in meteorites and are challenged to name the odor of which they are smelling. With the help of pictures illustrating shapes and 3-D models, the hands-on activity helps participants experience a specific structure-smell relationship that serves to represents how chemical structure is intimately tied to reactivity and interactions in biology. This relationship can be further extended to introduce the concept of chirality, a property that many organic molecules can exhibit by existing in two mirror image forms, called enantiomers. To illustrate the structural significance between mirror image compounds, two odorant enantiomers are presented to participants for a smell observation. The difference in odor is readily detected between the molecules even though they appear nearly identical. Participants are then introduced to how this property is related to a fundamental signature of life, known as homochirality, where the selection of one mirror image over the other is used in the construction of biological molecules and may have its roots in the origin of life itself. Lastly, we mention that meteorites may also help provide clues to questions surrounding the origin of homochirality given that reports of unequal amounts of enantiomers of certain classes of compounds, such as amino acids and sugar acids, have been detected in meteorites (2, 3).

Figure 1. An astrobiology outreach activity at the Ames Mini-Open House on Sep 22, 2017.

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Circular Dichroism-Thermal Lens Microscopy: A New Approach to Life Detection

Hiroshi Imanaka[1,2], Richard Quinn[1], Chris McKay[1]

[1] NASA Ames Research Center, [2] SETI Institute

The search for signatures life in extraterrestrial environments, including Mars, Europa, and Enceladus, is a high priority NASA science goal. However, most chirality based life detection methods need complicated sample preparation and require making a priori assumptions about chemical identity of the biomarkers that may be present in an exploration environment. For the detection of unknown biomarkers in the extraterrestrial environments, a robust direct chiral detection method with ultra high-sensitivity is needed.
Several groups are developing chiral separation and detection microchip devices, such as capillary electrophoresis coupled with laser-induced fluorescence (LIF). However, these are not inherently chiral sensitive detection methods; chiral separation is crucial to successful detection. Yet, chiral separations are difficult and poorly resolved multiple peaks often prevent reliable detection of chiral molecules.

We have been developing a circular dichroism–thermal lens microscope (CD-TLM) at ARC. This instrument is based on the photothermal lens effect combined with circular polarized light excitation. The importance of this approach is that it doesn't require chiral separation to independently measure the presence of both the left- and right-handed form of target molecules. It is a non-destructive analytical technique with ultra-high-sensitivity and is suitable for combination with other instruments. This CD-TLM method would provide a new complementally tool to the search for homo-chiral biosignatures from trace amount of samples in future solar system explorations.

PRODUCTION AND PRESERVATION OF LIPID BIOMARKERS BY IRON-OXIDIZING CHEMOLITHOTROPHS IN CIRCUMNEUTRAL IRON DEPOSITS.

E. T. Kelly[1], M. N. Parenteau[2], M. B. Wilhelm[2], A. F. Davila[2],R. C. Quinn[2], L. L. Jahnke[2], F. Rull[3], J.A. Sanz-Arranz[3], A. Sansano[3], [1]SETI Institute, Mountain View, CA 94043 (Erin.T.Kelly@nasa.gov); [2]Space Science and Astrobiology Division, NASA Ames Research Center, Moffett Field, CA 94035; [3]Unidad Asociada UVA-CSIC CAB, Paseo de Belén 5, Universidad de Valladolid, 47011 VALLADOLID (Spain).

Introduction: Data collected by the Mars Science Laboratory (MSL) and Mars Exploration Rover (MER) missions from the surface of Mars have provided (and continue to provide) mineralogical insights regarding the redox cycling of iron. Recent observations made by the MSL *Curiosity* rover have revealed ancient martian sedimentary deposits that experienced a small degree of Fe(II) oxidation (and thus, less acidity generated), allowing more benign – low salinity and circumneutral pH conditions to persist [1, 2, 3, 4].

We are studying circumneutral iron springs in Yellowstone National Park as an analog for circumneutral iron settings on Mars. We are examining the production and preservation of lipid biomarkers by chemolithoautotrophs, which oxidize Fe(II) to power their metabolism. Microbial communities such as these could have been operating on early Mars.

Results: We analyzed the lipid composition of two samples of flocculent biofilm containing chemolithoautotrophs such as *Leptothrix* and *Gallionella* collected from iron seeps at Chocolate Pots Hot Springs in Yellowstone. We extracted the lipids using solvents, separated them using thin layer chromatography, and analyzed them on a gas chromatograph-mass spectrometer (GC-MS). The dried biofilms were also analyzed using Raman spectroscopy. The samples were analyzed with a European Space Agency ExoMars flight prototype (the RLS Simulator) at UVa-CSIC-CAB Associated Unit. The aim was to compare the types of information revealed by GC-MS and the Raman ExoMars instrument**.**

Fatty acids. The chemolithoautotrophs grew in temperature ranges of 10 to 37^{o}C. The major fatty acids found in the higher temperature sample indicated the sample was dominated by chemotrophic iron-oxidizers such as *Leptothrix* [5]. Diagnostic biomarkers of these sheathed bacteria included hexadecanoic acid, cis-9-hexadecanoic acid, and oxadecanoic acid, all of which were dominant in the sample [5]. While present in lower abundance, unsaturated heptadecanoic acids and iso-heptadecanoic acid were also present in the higher temperature sample, indicating the presence of sulfate reducing bacteria. Wax esters, a diagnostic lipid biomarkers for green nonsulfur filamentous anoxygenic phototrophs (FAPs) (*Chloroflexus* and *Roseiflexus* spp.), were absent from both samples. However, the diversity of unsaturated heptadecanoic acid and high relative abundance of cis-9-octadecanoic acid and 9,12 octadecanoic acid implicate the presence of cyanobacteria in both samples, with a stronger relative presence in the cooler sample. Poly-unsaturated eicosanoic acid and docosanoic indicate possible contamination of the sample with detrital plant material.

Alkanes. Both samples were dominated by straight chain hydrocarbons, with midchain branched alkanes present. Monomethyl alkanes and heptadecanes were present in both samples, though in higher relative abundance in the cooler sample. These compounds are considered biomarkers for cyanobacteria [6,7].

Surprisingly, the lipid biomarkers resisted the earliest stages of microbial degradation and diagenesis to survive in the Fe oxides beneath the mats, though hydrocarbon signatures did show signs of degradation. Understanding the potential of particular sedimentary environments to capture and preserve fossil biosignatures is of vital importance in the selection of the best landing sites for future astrobiological missions to Mars. This study explores the nature of organic degradation processes in Fe(II)-rich groundwater springs— environmental conditions that have been identified as highly relevant for Mars exploration.

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Examining the evolution of oxygenic photosynthesis on the early Earth

Niki Parenteau[1], Linda L. Jahnke[1], Sherry Cady[2], and Beverly K. Pierson[3]

[1]NASA Ames Research Center, Mountain View, CA 94035
[2]Pacific Northwest National Lab, Richland, WA 99354
[3]University of Puget Sound, Tacoma, WA 98416

The evolution of the atmosphere, ocean, and microbial life on the early Earth were inextricably linked. The evolution of oxygenic photosynthesis and the resulting oxygenation of the atmosphere and oceans was arguably one of the most important events in the history of the young planet.

While modern cyanobacteria produce oxygen as a waste product from the oxidation of water, it may not have always been so. There is a large difference in the redox potentials between water used as an electron donor by cyanobacteria and hydrogen commonly used by the more ancient anoxygenic photosynthesis. Members of our group have speculated that an intermediate reductant such as Fe(II) could have bridged the gap and acted as a transitional electron donor before water. The widespread abundance of Fe(II) in Archean and Paleoproterozoic ferruginous oceans would have made it particularly suitable as an electron donor for photosynthesis. Therefore, iron-dependent photosynthesis using one photosystem in cyanobacteria may have been an important step in the evolution of oxygenic photosynthesis.

We have been searching for modern descendants of such an ancestral "missing link" cyanobacterium in a high-iron thermal springs. In our physiological ecology study of the cyanobacterial mats, we have found evidence that this type of metabolism is occurring *in situ* using carbon-14 bicarbonate uptake experiments and autoradiography. We have detected a stimulation of C-14 uptake in the presence of Fe(II) in lower light adapted cyanobacteria that inhabit the lower end of the photic zone in microbial mats. We are currently probing the metagenomic data obtained from the JGI Yellowstone National Park Community Sequencing Project for the molecular underpinnings of this process.

A complimentary study of the microbial biosignatures produced in these mats revealed diagnostic lipid biomarkers for cyanobacteria: mid-chain branched mono- and dimethylalkanes and, most notably, 2-methylhopanoids. This is the first documentation of 2-methylhopanoids in a modern iron-mineralized cyanobacterial mat where the cyanobacteria have been shown to grow anoxygenically using Fe(II) as an electron donor for photosynthesis.

THE IMPACT OF RNA LENGTH ON EVOLUTION OF RNA FUNCTION

Milena Popović[1,2], Alexander Ellingson[1,2], Theresa Chu[1,2], Andrew Plebanek[1,3], Chenyu Wei[1,3], Andrew Pohorille[1,3], and Mark Ditzler[1].

[1]Exobiology Branch, NASA Research Center, Mail Stop 239-4, Moffett Field, CA 94035; [2]Blue Marble Space Institute of Science, Seattle, WA 98145, [3]Department of Pharmaceutical Chemistry, UCSF; milena.popovic@nasa.gov, andrew.pohorille@nasa.gov, chenyu.wei@nasa.gov, mark.a.ditzler@nasa.gov.

Ribonucleic acids (RNA) are widely considered to be early, if not earliest molecules to transmit heritable information and perform catalysis. The length of the earliest evolving RNA molecules is thought to have been limited and increasing over time. Combined phylogenetic and structural evidence suggests that complex modern RNAs share structure with their much shorter ancestral RNA. Understanding the role of RNA in the origin and evolution of life, therefore, requires an understanding of the role of length in evolution of RNA function. We evolved populations of ligase ribozymes of two lengths: a population of short (20N) and long (80N) ligases, with fully randomized sequence of respective length N. We analyzed the evolved populations by combining high throughput sequencing data and comparative sequence and structure analysis. One of the main questions we wanted to answer by evolving both short and long ligases in parallel is how the additional sequence is utilized by catalytic RNA. We observe evolution of recurring structures among the populations of short and long ribozymes. We detect both short and long ligase ribozymes that favor the same ligation junction and form identical secondary structures surrounding them. Structures evolved in the 20N population are also present as components of larger structures in the 80N population, suggesting a role for growth through elaboration upon existing structure- “accretion”. We tested the activity of these ribozymes and observe a consistent increase in activity as a function of length. Moreover, we observe a length-activity correlation across nine orders of magnitude in activity among multiple ligase ribozymes evolved under a range of conditions from different laboratories. This length-activity relationship can serve as a constraint on the catalytic roles assigned to RNA in models of early evolution. We are currently evolving ligase ribozymes to test how continued growth impacts on activity of previously evolved ligases. We will test whether additional sequence contributes to structure growth through elaboration upon structural solutions available to short RNA or results in entirely new structures, inaccessible to short RNA. We hypothesize that the additional sequence will have an impact on activity proportional to the length of the RNA. Understanding how polymer length impacts evolution provides both insight into early evolution and provides guidance to the interpretation of the molecular record present in modern RNA structures.

MAPX-PIXE: A Full Field Micro X-Ray Fluorescence Imager for Astrobiology Applications on Ocean Worlds. R. C. Walroth,[1] D.F. Blake,[1] P. Sarrazin,[2] K. Thompson,[2] T. Bristow[1] and S. A. Meursing[1] [1]Exobiology Branch, MS 239-4, NASA Ames Research Center, Moffett Field, CA 94035 (richard.c.walroth@nasa.gov), [2]SETI Institute, Mountain View, CA 94043.

Introduction: Investigations of Ocean Worlds and other bodies as potential habitats for life require a knowledge of the mineralogy and elemental chemistry at the surface [1]. The Mapping X-ray Fluorescence Spectrometer (MapX) employs XRF at the micrometer scale (μXRF) to obtain such information [2]. MapX-PIXE has been designed for use with radioisotope sources that will emit both α and γ radiation. The γ radiation will induce XRF from heavy elements, while α particles will be able to induce XRF from lighter elements *via* particle induced X-ray emission (PIXE). Thus, MapX-PIXE will be capable of imaging both heavy elements for mineralogy and dissolved ion characterization and light elements for possible identification of biological material.

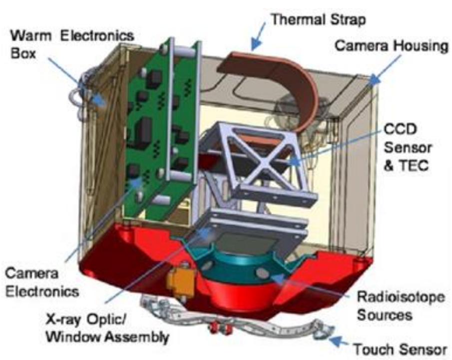

Figure 1. Proposed design for a MapX-PIXE instrument.

MapX Prototypes to Date: MapX is a full-field XRF imager which employs a CCD detector operated in single photon counting mode. MapX combines this CCD with a micro-pore optic (MPO) which focuses X-rays 1:1 onto the CCD. The resulting instrument is capable of producing μXRF maps with a resolution of ~100 μm. Data is currently being collected using two prototypes employing X-ray tube sources, MapX-II and MapX-III, which are at TRL3 and TRL4 respectively.

The MPO/CCD geometry has significant advantages over other μXRF systems. MapX has no moving parts. Further, the MPO provides a greater depth of field than instruments which employ polycapillary optics. MapX has a measured depth of field of approximately 10 mm, which means that rough, unprepared surfaces can be imaged with minimal loss of resolution.

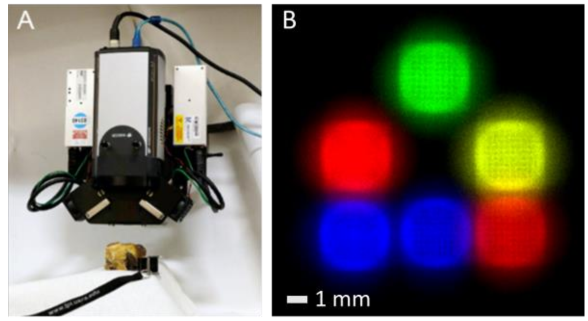

Figure 2. A) MapX-II prototype employing two X-ray tubes and a commercial CCD. B) Mesh grid targets demonstrating spatial resolution and sensitivity to element identity. Cu in red, Ti in blue, Fe in green, and Ni in yellow.

Employing Radioisotope Sources: So far, MapX has been developed with X-ray tube sources which efficiently excite elements heavier than Ne. Using fundamental parameters methods it is possible to calculate the overall composition in terms of weight percent for heavy elements without directly measuring the light elements. However, detecting life or its precursors on Ocean Worlds will require the detection and mapping of C and N. To this end, MapX-PIXE will employ ^{244}Cm which emits 14 keV and 18 keV γ-rays as well as 5.8 MeV α-particles [3]. The γ-rays efficiently excite heavy elements ($20 < Z < 30$) similarly to X-ray tubes, while α-particles excite lighter elements ($\sim 6 \leq Z < 19$) *via* PIXE. GEANT4 simulations demonstrate the increased signal from light elements when using ^{244}Cm compared to X-ray tubes [4]. A ^{244}Cm equipped MapX-PIXE instrument will be smaller, less complex and more robust than an X-ray tube based instrument. Radioisotope-based XRF instruments have been employed on the MER and MSL rovers, demonstrating their feasibility in flight [3].

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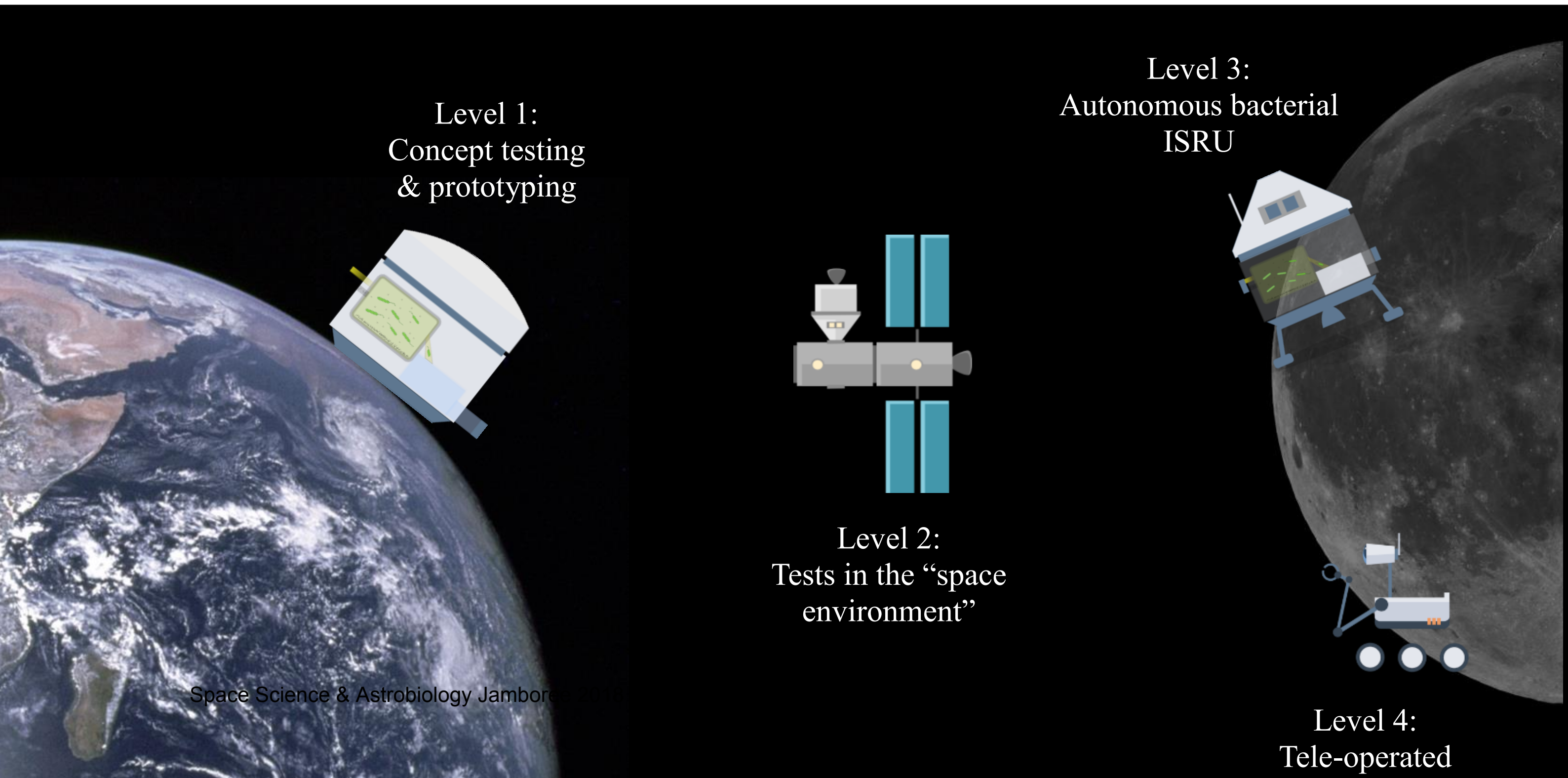
Novel possibilities in material extraction enabled through biological in situ resource utilization (ISRU)

Authors: Benjamin Lehner, Anne S. Meyer, Stan J.J. Brouns* and Lynn Rothschild*

Abstract: In situ resource utilization (ISRU) is increasingly acknowledged as an essential part of sustainable space exploration. Even with the current trend of decreased launching costs and reusable rockets, the ultimate goal to increase human activities in space must be the usage of resources found at the destination. Typical approaches towards ISRU are often constrained by the mass and energy requirements of transporting processing machinery, such as rovers and bulky reactors, and a vast amount of consumables needed. A self-reproducing biological ISRU system with minimal requirements would avoid or complement many crucial issues. Microbiological systems are promising candidates for several approaches including the purification, alteration, and extraction of materials from the lunar regolith. The presentation will show current efforts in the sector of material extraction, mainly iron and silicon, combined with an end-to-end mission architecture (sketch below), which also includes limitations due to biological contamination and the need for a constant nutrient supply. Finally concluding, that the development of biological ISRU techniques can be an effective new means of promoting more efficient, sustainable space exploration.



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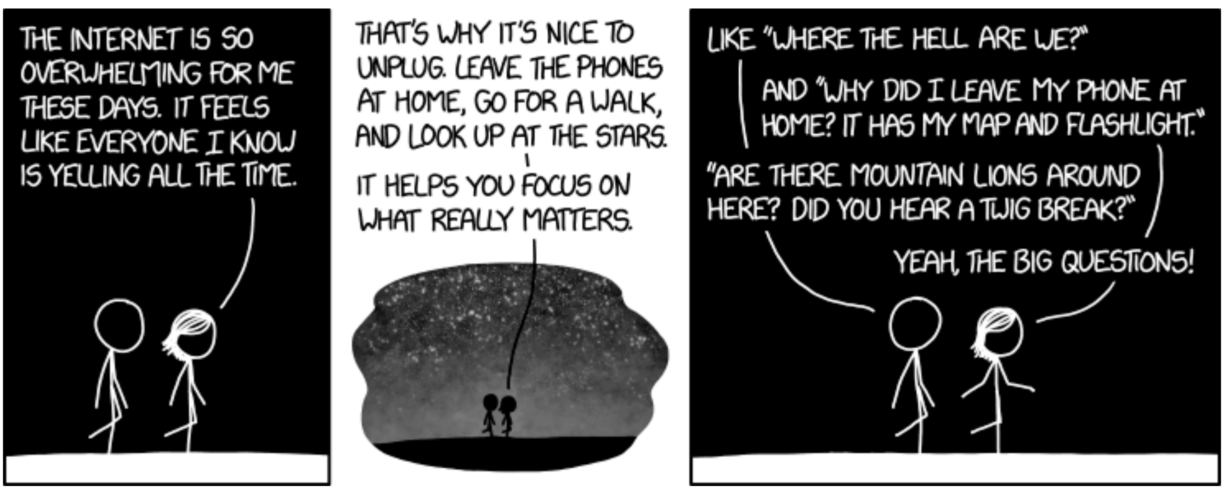


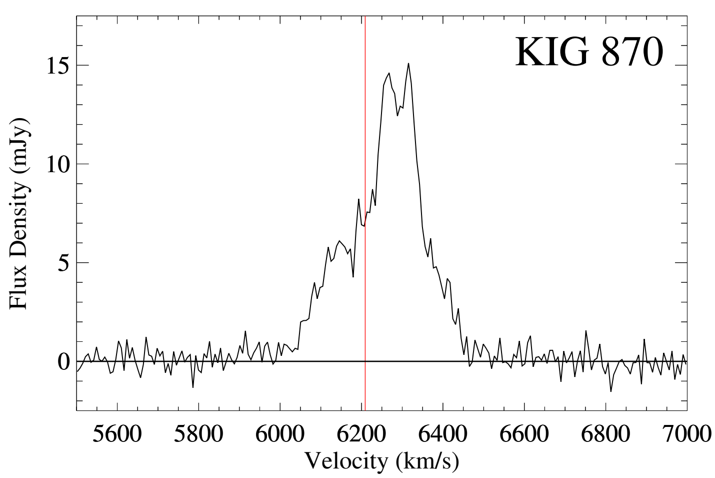
https://xkcd.com/1947/

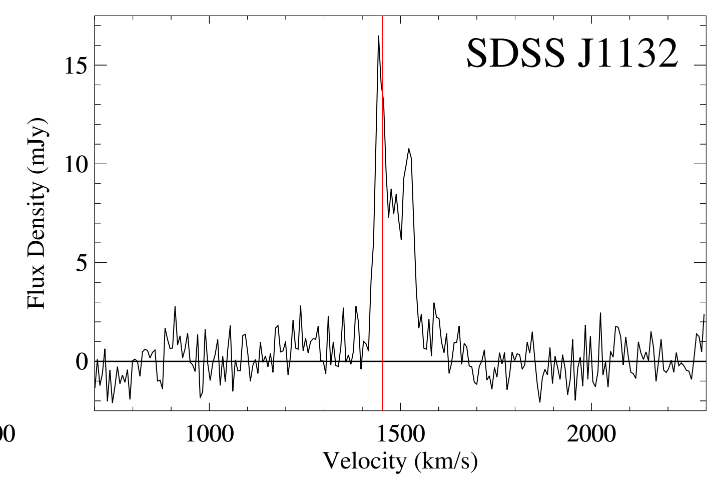
Astrophysics

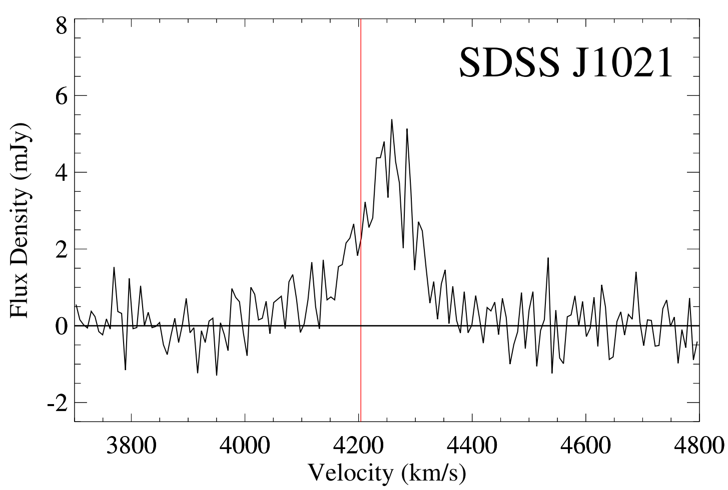
Title: An HI Survey of Extremely Isolated Early-type Galaxies

Authors: Trisha Ashlev. Pamela Marcum, and Michael Fanelli

Abstract: We present the results from an HI survey of extremely isolated early-type galaxies (IEGs) conducted using the Robert C. Byrd Green Bank Telescope (GBT). **IEGs are a rare subgroup of early-type galaxies (ETGs) that enable unique empirical tests of competing galaxy formation and evolution models.** The IEGs in our study are isolated to within 2.5 Mpc from other galaxies with luminosities brighter than M_V=-16.5. These galaxies have been studied previously at optical wavelengths to characterize the stellar populations; HI measurements reveal, for the first time, the properties of their neutral gas content. Seven of the twelve IEGs in the sample are detected in HI. The detected galaxies exhibit HI line profiles with a range of properties, including: single Gaussian-like peaks, separate double peaks, asymmetric HI profiles, and double horn profiles. The different HI line profile shapes indicate that the gaseous disks of these galaxies likely have a variety of shapes, including: thin disks with differential rotation and thick disks with solid-body-like rotation (e.g. dwarf galaxy disks).







Dynamics of Pure and N-substituted Cyclic Aromatic Hydrocarbon Formation in the Gas-Phase

Partha P. Bera[1,2], Tamar Stein[3], Martin Head-Gordon[3], and Timothy J. Lee[1]

1. Space Science and Astrobiology Division, NASA Ames Research Center
2. Bay Area Environmental Research Institute
3. University of California – Berkeley

E-mail: Partha.P.Bera@nasa.gov

Abstract:

The processes by which complex organic molecules including large polycyclic aromatic hydrocarbons, known to be ubiquitous in the interstellar medium and accounting for a significant portion of total carbon in the universe, is thus far unknown. Organic molecules are found in diverse astrophysical environments, most notably in molecular clouds. Molecular ions, including positive and negative ions, are abundant in the high radiation fields present in star forming regions. Barrierless ion-molecule interactions may play a major role in guiding molecules towards each other and initiating reactions. We study neutral as well as ion-neutral condensation pathways to determine whether they are a viable means of forming large pure hydrocarbon molecules, nitrogen-containing carbonaceous chains, and cyclic compounds, by employing a variety of quantum chemical methods including coupled cluster and density functional theory methods. Where possible, the results from our calculations are compared with the results from experimental studies such as plasma discharge and ion-mobility experiments. We have investigated the process of growth, structural features, nature of bonding, reaction mechanisms, and spectroscopic properties of the ensuing products after pairing carbon, hydrogen, and nitrogen-containing precursors. Ab-initio molecular dynamics trajectory studies of the ion-neutral association pathways involving pure-carbon and nitrogen-containing precursors spanning several nanoseconds at various temperatures reveal interesting details about the cyclic molecule formation process, and also their limitations. We found that hydrocarbon reactants with suitable starting geometries and specific stoichiometric compositions prefer cyclic molecule formation rather than chains. Some of the association products we investigated have large oscillator strengths for charge-transfer type electronic excitations in the near infrared and visible regions of the electromagnetic spectrum.

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Tracing the Charge Balance of Polycyclic Aromatic Hydrocarbons Across a Reflection Nebula, an H II-region and a Planetary Nebula

Christiaan Boersma[1,2], Louis J. Allamandola[1,3], and Jesse D. Bregman[1,3]

1. NASA Ames Research Center — 2. SJSURF — 3. BAERI

Polycyclic aromatic hydrocarbons (PAHs) are an important constituent of interstellar dust. Intermediate in size between molecules and particles, PAHs have characteristics of both. This unique property, coupled with their spectroscopic response to changing conditions and the ability to convert ultraviolet to infrared (IR) radiation, makes them powerful probes of astronomical objects at all stages of the stellar lifecycle. PAH emission can dominate as much as 20% of the total IR luminosity in the many Galactic and extragalactic objects where they are seen, and they are thought to hold up to 10-15% of *all* cosmic carbon. Due to their omnipresence and stability, PAHs play important roles in many astronomical environments and a defining role in the star- and planet formation process; and perhaps even in the origin of life itself. The *Spitzer*-IRS spectral maps of a reflection nebula (NGC 7023), an H II-region (M17) and a planetary nebula (NGC 40) are analyzed using the data and tools made available through the NASA Ames PAH IR Spectroscopic Database (PAHdb; www.astrochemistry.org/pahdb/).

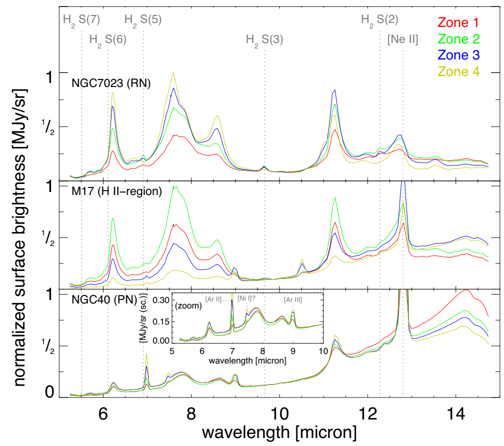


Figure 1: *Average 5.2-14.5 μm Spitzer-IRS spectra for four zones identified in each target through Hierarchical Clustering.*

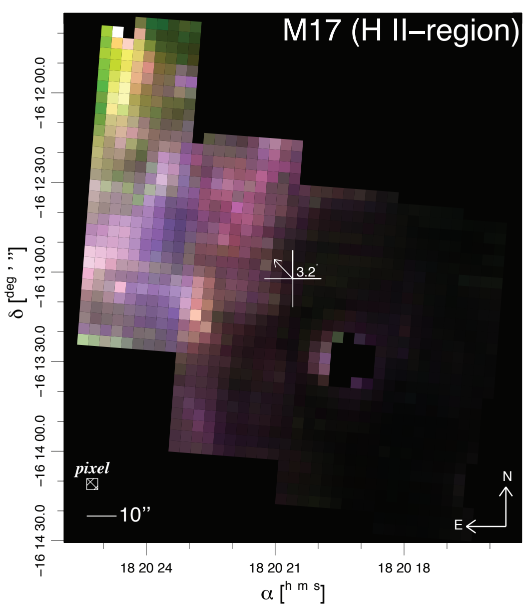


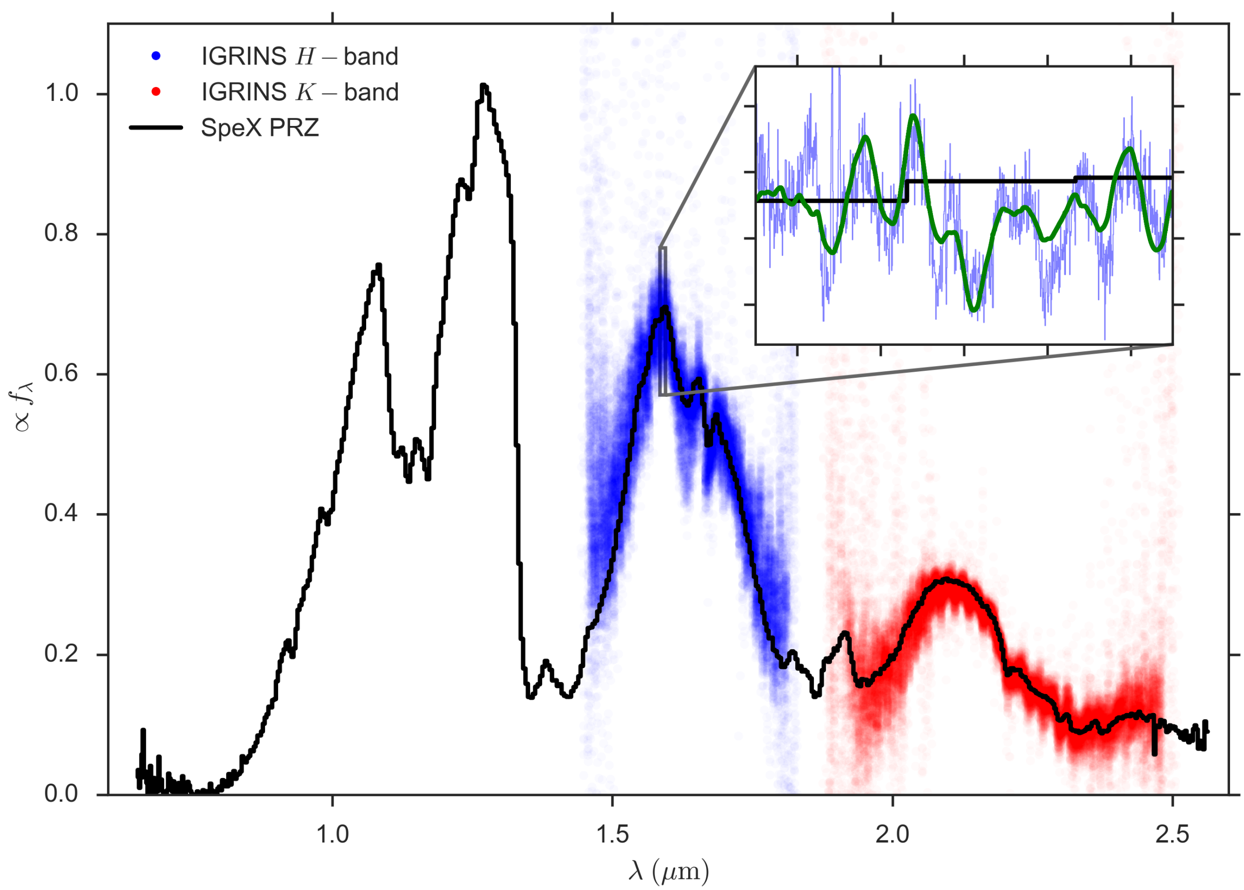
Figure 2: *Three-color composite constructed from the quantitative PAHdb charge breakdown. The contribution from PAH anions, neutrals and cations are shown in red, green and blue, respectively.*

The PAH emission spectrum in these maps is broken down, pixel-by-pixel, into *quantitative* PAH charge contributions using a database-fitting approach. The *quantitative* breakdown results are used to calibrate the *qualitative* results derived using the traditional PAH band strength approach, which interprets particular PAH band strength ratios as *qualitative* proxies for the charge balance of the PAH population. The *quantified* charge proxies are linked to the PAH ionization parameter, which connects the charge balance to the gas temperature, electron density and the strength of the radiation field at each pixel across the emitting region, not only tracing changing conditions across each nebula, but also tracing the evolution of carbon within these different astronomical objects.

Inferring fundamental properties of young stars and brown dwarfs

Michael Gully-Santiago

Czekala and collaborators (2015) developed a modular spectral inference framework aimed at deriving accurate fundamental properties of planet-host stars from observed spectroscopy. Spectral inference---also called "retrieval" analysis---is an increasingly practical Bayesian system for delivering both best fit values and the probability density cloud of uncertainty in the best fit values. The framework solves for all stellar intrinsic (e.g. Teff, logg, [Fe/H], [alpha/Fe]) and extrinsic (RV, vsini, solid angle, Av) parameters simultaneously, encapsulating degeneracies among parameters. The Czekala et al. framework resolved multiple practical barriers in the comparison of pre-computed synthetic spectral models to observed spectra, for example discretization uncertainty attributable to coarsely sampled model grids and residual correlation structure common in oversampled spectrographs. Over the last year, I have extended the open source Python implementation, Starfish, to support additional separable physical model components. The extensions include circumstellar disk emission, starspot emission, and binarity. I have also demonstrated the the framework on the complex spectra of brown dwarfs by consuming a large new model grid from Marley and collaborators. The Marley model grid extends from 200 K to 2400 K in effective temperature, making this technique amenable to the characterization of the spectra of directly imaged exoplanets with JWST or extremely large telescopes. These extensions and demonstrations make Starfish an excellent choice for robust characterization of planet host stars, substars, and planets in almost any environment.



Poster Title: PAH Infrared Spectroscopy in the JWST Era: a computational and laboratory study

Authors: Alessandra Ricca[1,2], Joseph Roser[1,2], Jean Chiar[1,3], Els Peeters[4], Xander Tielens[5]
Affiliations: (1) SETI Institute (2) NASA-Ames Research Center (3) Diablo Valley College (4) University of Western Ontario, Canada (5) Leiden University

Abstract: The Infrared Space Observatory and Spitzer Space Telescopes have shown that the mid-IR emission spectrum of the interstellar medium is dominated by strong bands at 3.3, 6.2, 7.7, 8.6, 11.3 and 12.7 microns superimposed upon broad underlying plateaus generally attributed to PAHs, PAH clusters and very small grains. Despite the limited spectral and spatial resolution of these data, detailed analysis has revealed that each band is, in fact, a blend of multiple emission features. Subtle variations in the band blending can be detected even for spectra measured at different positions within a single astronomical source. These variations can be seen to arise from multiple PAH and PAH-related carriers that are each responding differently to the local physical conditions. The James Webb Space Telescope has near-IR and mid-IR instruments, NIRSpec and MIRI, with an extremely high spectral resolution, spatial resolution, and sensitivity that will revolutionize infrared astronomy. These instruments will provide spatial maps on a sub-arcsecond scale with an unprecedented level of spectral detail, allowing detailed study of the interrelationship of the individual components within each emission band. This will provide a critical insight into the molecular characteristics of the emitting species and their (photo)chemical evolution in space.

Exploitation of these astronomical spectra requires infrared data on potential emitting species that fully account for all astrophysically relevant materials. We have undertaken a combined program of computational modeling and laboratory experiments to be conducted at NASA-Ames Research Center to calculate the IR spectra of isolated as well as clustered neutral and charged PAHs containing up to 150 carbon atoms and with a wide variety of structures ranging from compact with straight edges, compact with bay regions, non-compact with various shapes and erosion sites, and PAHs containing defects. These theoretical data are be validated by a dedicated laboratory study of neutral and cationic PAH species containing up to 70 carbon atoms and their clusters. The IR absorption spectra are used to calculate emission spectra that can be directly compared to existing Spitzer Infrared Spectrograph (IRS) maps of reflection nebulae (RNe) and star forming regions and future astronomical observations obtained by NIRSpec and MIRI on JWST, as shown in Figure 1.

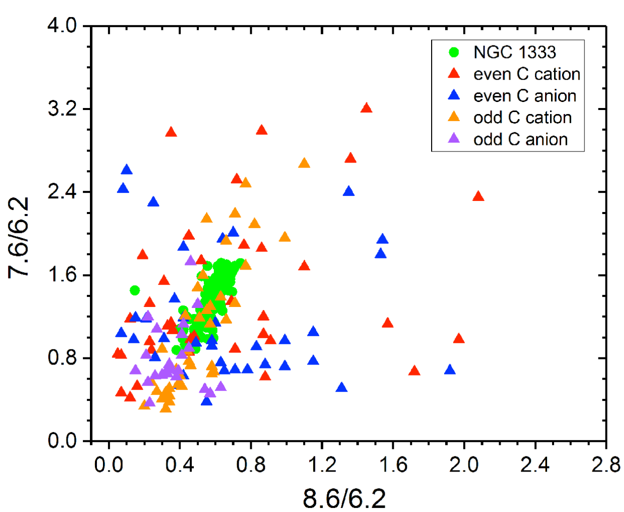


Figure 1. Comparison of the intensity ratios of even-carbon PAH cations (red triangles) and anions (blue triangles), and odd-carbon PAH cations (orange triangles) and anions (purple triangles), computed for an excitation of 8 eV and after applying a redshift of 15 cm^{-1}, with observations (green circles) of the RNe NGC 1333.

The Mid-Infrared Imager/Spectrometer/Coronagraph Instrument (MISC) for the Origins Space Telescope

Thomas L. Roellig[1], Itsuki Sakon[2], Kimberly Ennico[1], and the MISC Instrument Study Team

1. NASA Ames Research Center, 2. The University of Tokyo

Abstract

The Origins Space Telescope (OST) is one of four potential flagship missions that have been funded by NASA for study for consideration in the upcoming Astrophysics Decadal Review expected in 2020. The OST telescope will be up to 9.3 meters in diameter, cooled to ~4K, and the mission will be optimized for efficient mid and far-infrared astronomical observations. An initial suite of five focal plane instruments are being baselined for this observatory. The MISC instrument will observe at the shortest wavelengths of any of these instruments, ranging from 5 to 38 microns, and consists of three separate optical modules providing imaging, spectroscopy, and coronagraph capabilities. The imaging camera covers a 3' x 3' field with filters and grisms from 6-38 microns. The spectrometers have spectral resolving powers R~1,000 from 9-38 microns (with a goal of 5-38 microns) and R~25,000 for 12-18 and 25-36 microns. The coronagraph covers 6-38 microns. There is a special densified pupil spectrometer channel that would be used for R~100-300 exoplanet transit and emission spectroscopy from 6-26 microns with very high spectro-photometric stability. As the shortest wavelength focal plane imager the MISC instrument will also be used for focal plane guiding as needed for the other OST science instruments.

The COsmic SImulation Chamber (COSmIC) at NASA Ames: a Multipurpose Laboratory Astrophysics Facility

Farid Salama[1], Ella Sciamma-O'Brien[1, 2] and Salma Bejaoui[1]
[1]NASA Ames Research Center, Moffett Field, CA, [2]Bay Area Environmental Research Institute, Moffett Field,, CA.

We describe the characteristics and the capabilities of the laboratory facility, COSmIC, that was developed at NASA Ames to generate, process and analyze interstellar, circumstellar and planetary analogs in the laboratory[1]. COSmIC stands for "Cosmic Simulation Chamber" and is dedicated to the study of neutral and ionized molecules and nanoparticles under the low temperature and high vacuum conditions that are required to simulate various space environments such as diffuse interstellar clouds, circumstellar outflows and planetary atmospheres. COSmIC integrates a variety of state-of-the-art instruments that allow forming, processing and monitoring simulated space conditions in the laboratory. The COSmIC experimental setup is composed of a Pulsed Discharge Nozzle (PDN) expansion, that generates a plasma in the stream of a jet-cooled supersonic expansion (50-150 K), coupled to two high-sensitivity-, complementary *in situ* diagnostics: a cavity ring down spectroscopy (CRDS[2]) and laser induced fluorescence (LIF[3]) systems for photonic detection, and a Reflectron Time-Of-Flight Mass Spectrometer (ReTOF-MS) for mass detection in real time[4].

Recent results obtained using COSmIC in many fronts will be highlighted. In particular, the progress that has been achieved (i) in the domain of the diffuse interstellar bands (DIBs [5]) and the ESO Diffuse Interstellar Bands Large Exploration Survey, EDIBLES [6, 7], (ii) in monitoring, in the laboratory, the formation of circumstellar dust grains [8] and (iii)in the study of planetary atmosphere aerosols [9, 10, 11] from their gas-phase molecular precursors. Plans for future laboratory experiments on interstellar and planetary molecules and grains will also be addressed, as well as the implications of the studies underway for astronomical observations (EDIBLES) and space mission (HST, JWST, SOFIA, ...) data analysis.

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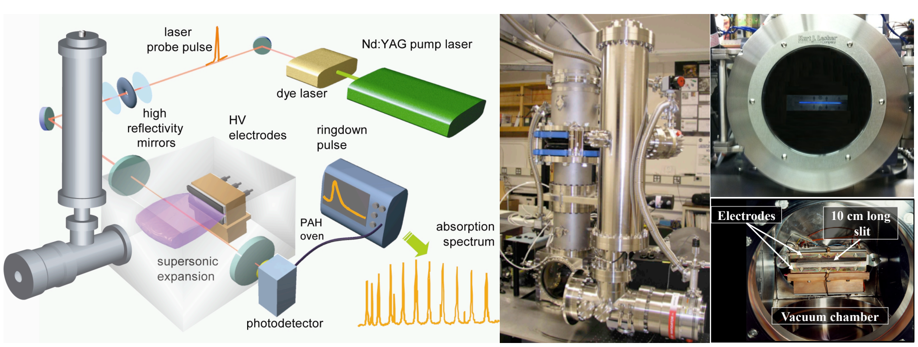


The NASA Ames Cosmic Simulation Chamber:

The astronomical 7.7 µm polycyclic aromatic hydrocarbon complex: *Insights from the NASA Ames PAH Infrared Spectroscopic Database*

Matthew J. Shannon[1,2], Christiaan Boersma[2,3]
1—USRA, 2—NASA Ames Research Center, 3—SJSURF

We present insights into the behavior of the astronomical 7.7 µm polycyclic aromatic hydrocarbon (PAH) emission complex as gleaned from analyzing synthesized spectra, utilizing the NASA Ames PAH IR Spectroscopic Database (www.astrochemistry.org/pahdb/; PAHdb). We specifically study the influence of PAH size, charge, aliphatic content and hetero-atom substitution on the profile and peak position of the 7.7 µm feature ($\lambda_{7.7}$). The 7.7 µm feature is known to vary significantly from object to object in astronomical observations (see Fig. 1): from class A in interstellar-type environments ($\lambda_{7.7} \sim 7.6$ µm) to class B in circumstellar-type environments ($\lambda_{7.7} \sim 7.8$ µm). A handful of objects exhibit a broad, redshifted peak known as class C ($\lambda_{7.7} \gtrapprox 8.0$ µm), or a flat plateau (class D). The origin of these variations is currently highly speculative.

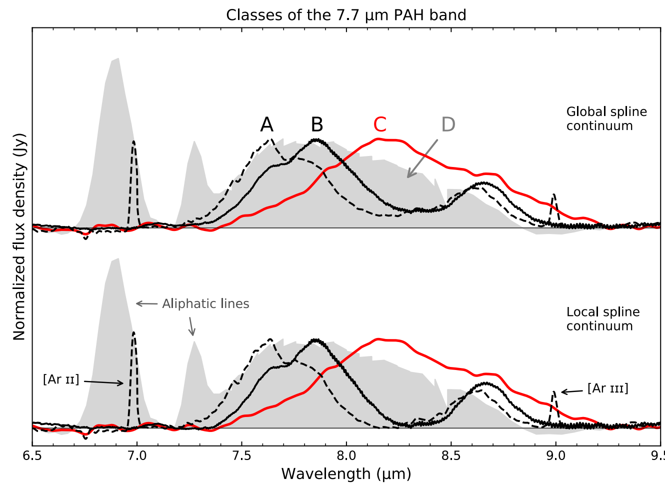


Figure 1. The four classes of the 7.7 µm PAH emission complex, which are linked to object type. The physical/chemical changes in PAH populations needed to explain these variations are currently largely unknown.

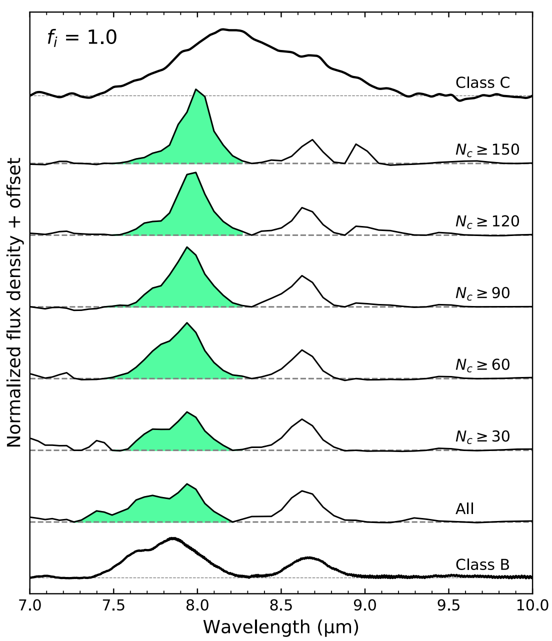


Figure 2. Synthetic spectra created using PAHdb (those with the shaded green bands) are compared to the astronomical templates of class B and C. Note the change of the PAH band profiles as the PAH sizes vary.

Our results indicate that PAH size is the largest driver of shifts in $\lambda_{7.7}$: relatively small PAHs are consistent with class A spectra and large PAHs are consistent with very red B spectra. As an example, we show some spectra synthesized using PAHdb in Fig. 2. In total, size can account for $\Delta\lambda_{7.7} \sim 0.4$ µm shifts, from 7.6 µm to nearly 8.0 µm, accounting for the class A→B transition. PAHs with aliphatic side groups or super-hydrogenated PAHs, of which PAHdb contains a modest amount, can produce redshifts typically around 0.15 µm, and changes in ionization fraction approximately 0.1 µm depending on species. Thus, within the limits of PAHdb, the class A→B transition is best explained with changes in PAH size distributions, with a relatively minor role assigned to aliphatic content and varying charge states. The addition of PAH species with a larger variation in sizes, edge structures and aliphatic content to PAHdb, and an emission model taking anharmonic profiles into account can put our findings on a stronger footing.

Title: Shaken Snow Globes: Kinematic Tracers of the Multiphase Condensation Cascade in Massive Galaxies

Authors: Pasquale Temi (NASA – Ames), Massimo Gaspari (Princeton University)

The objective of our investigations is to clarify the formation and evolution of multiphase gas in the atmospheres of massive galaxies at the centers of galaxy groups and clusters. Multiwavelength observations are crucial to our understanding of the physics of multiphase gas and in driving modeling of key astrophysical processes. 3D high-resolution magnetohydrodynamic simulations via high-performance supercomputing, are used to explore the full condensation cascade, from the hot (X-ray) phase to the warm (optical), cold (infrared), and molecular phase (radio).

In our latest work we propose a novel method to constrain turbulence and bulk motions in massive galaxies, groups and clusters, exploring both simulations and observations. As emerged in the recent picture of the top-down multiphase condensation, the hot gaseous halos are tightly linked to all other phases in terms of cospatiality and thermodynamics. While hot halos (10^7 K) are perturbed by subsonic turbulence, warm (10^4 K) ionized and neutral filaments condense out of the turbulent eddies. The peaks condense into cold molecular clouds (< 100 K) raining in the core via chaotic cold accretion (CCA). We show all phases are tightly linked via the ensemble (wide-aperture) velocity dispersion along the line of sight. The correlation arises in complementary long-term AGN feedback simulations and high-resolution CCA runs, and is corroborated by the combined Hitomi and new IFU measurements in Perseus cluster. The ensemble multiphase gas distributions are characterized by substantial spectral line broadening (100-200 km/s) with mild line shift. On the other hand, pencil-beam detections sample the small-scale clouds displaying smaller broadening and significant line shift up to several 100 km/s, with increased scatter due to the turbulence intermittency. We present new ensemble sigma_v of the warm H_{alpha}+[NII] gas in 72 observed cluster/group cores: the constraints are consistent with the simulations and can be used as robust proxies for the turbulent velocities, in particular for the challenging hot plasma (otherwise requiring extremely long X-ray exposures).

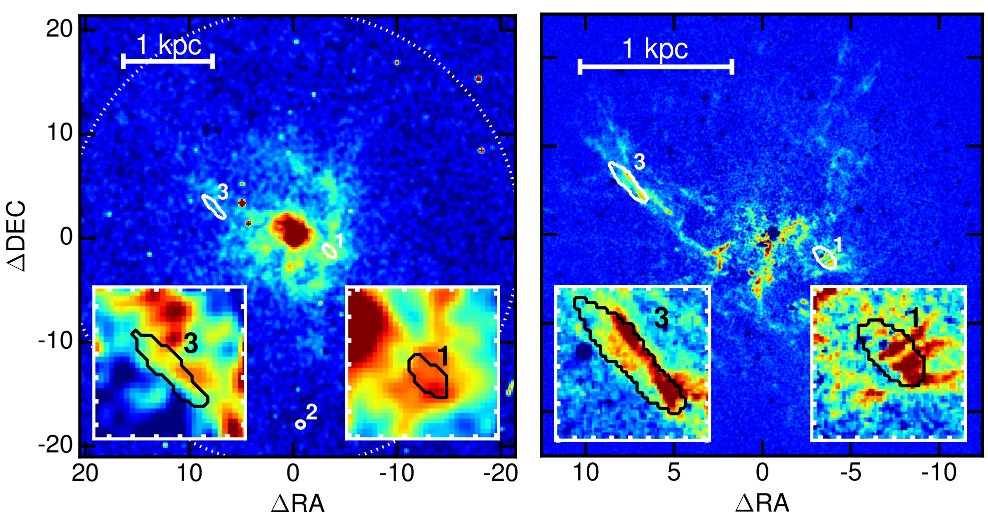
The objectives of this work are aligned with the on-going development of the *Arcus* X-Ray Grating Spectrometer Mission (Phase-A Midex Explorer). This investigation provides constraints on the fundamental interaction between massive black holes and galaxies via comparison of observational data with simulations.

This project made extensive use of the NASA Advanced Supercomputing (NAS) resources at NASA/Ames (Program SMD-16-7320, SMD-16-7321, SMD-16-7305).

Title: ALMA observations of molecular clouds in three group centered elliptical galaxies

Authors: Pasquale Temi (NASA – Ames), Alexandre Amblard (NASA – Ames)

This work presents new ALMA CO(2-1) observations of two well studied group-centered elliptical galaxies: NGC 4636 and NGC 5846. In addition, we include a revised analysis of Cycle 0 ALMA observations of the central galaxy in the NGC 5044 group that has been previously published. We find evidence that molecular gas, in the form of off-center orbiting clouds, is a common presence in bright group-centered galaxies (BGG). CO line widths are ≳10 times broader than Galactic molecular clouds, and using the reference Milky Way *XCO*, the total molecular mass ranges from as low as 2.6×105$M_{\odot}$ in NGC 4636 to 6.1×107$M_{\odot}$ in NGC 5044. With these parameters, the virial parameters of the molecular structures is ≫1. Complementary observations of NGC 5846 and NGC 4636 using the ALMA Compact Array (ACA) do not exhibit any detection. The origin of the detected molecular features is still uncertain, but these ALMA observations suggest that they are the end product of the hot gas cooling process and not the result of merger events. Some of the molecular clouds are associated with dust features as revealed by HST dust extinction maps suggesting that these clouds formed from dust-enhanced cooling. The global nonlinear condensation may be triggered via the chaotic turbulent field or buoyant uplift. The large virial parameter of the molecular structures and correlation with the warm/hot phase velocity dispersion provide evidence that they are unbound giant molecular associations drifting in the turbulent field, consistently with numerical predictions of the chaotic cold accretion process. Alternatively, the observed large CO line widths may be generated by molecular gas flowing out from cloud surfaces due to heating by the local hot gas atmosphere.

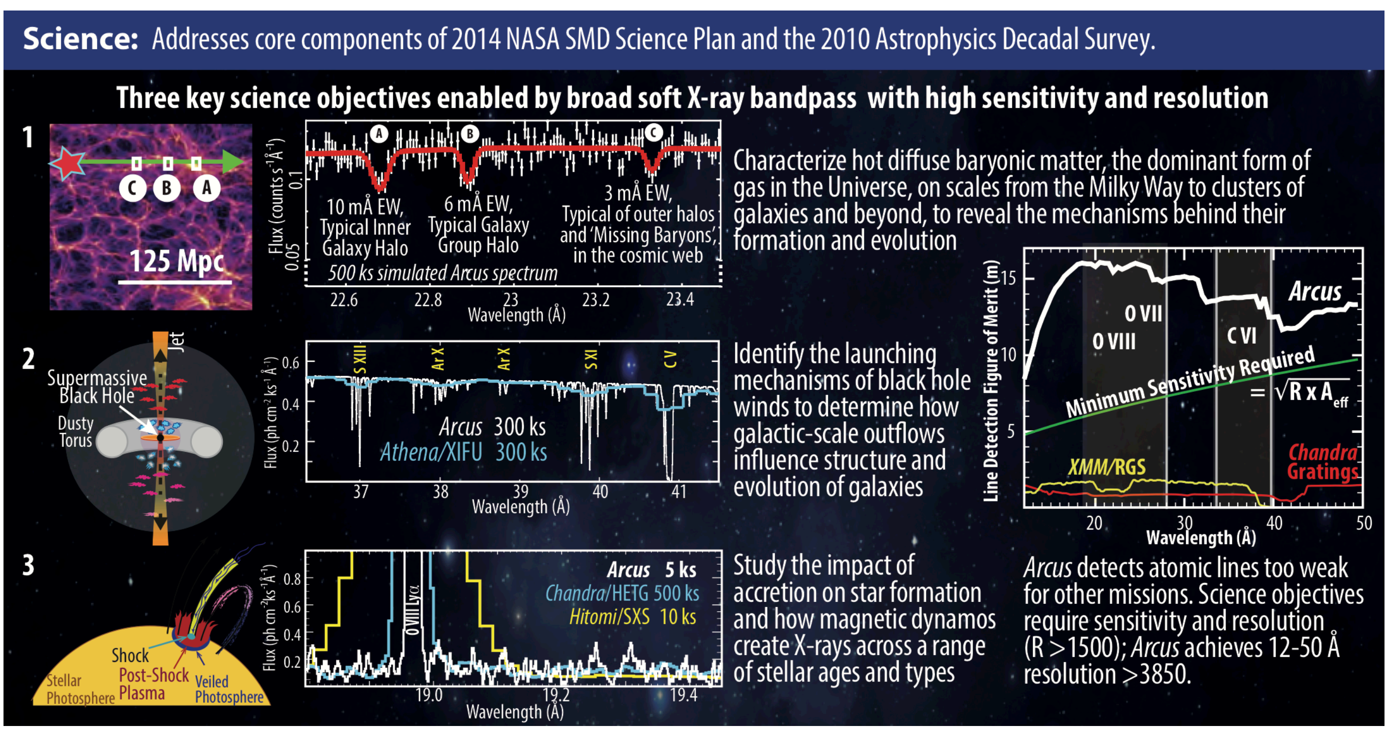


Images of NGC 5846 showing detected CO(2-1) clouds projected against an optical Hα+N[II] emission (left) and a dust starlight extinction image (right). Color sequence (blue → green → yellow → red) indicates increasing Hα+[NII] and dust. CO clouds, indicated with black (in the insert) and white contours, are defined as the area where the emission line signal-to-noise is greater than 4. Clouds #1 and #3 are somewhat resolved and extend about 1.2′′ and 2.9′′. Note that cloud #3 (see enlarged insert) is aligned almost exactly along a dust filament, and coincides with knots and filamentary structures in the Hα+[NII] emission. Cloud #1 also coincides with Hα+[NII] emission and dust extinction, but other similar dusty regions were not detected in CO(2-1). Cloud #2 is not associated with detectable optical emission and out of dust extinction map FOV. The white dashed circle in the Hα+N[II] emission map identifies the field of view of the ALMA primary beam.

Title: *Arcus* - The X-ray Grating Spectrometer Explorer

Authors: Pasquale Temi (NASA – Ames) and the ARCUS Team

Arcus is a NASA/MIDEX Explorer mission that has been selected for Phase A study in August 2017. It is a free-flying satellite mission that will enable high-resolution soft X-ray spectroscopy (8-50Å) with unprecedented sensitivity – effective areas of >3500 sq cm and spectral resolution >2500. The Arcus key science goals are (1) to determine how baryons cycle in and out of galaxies by measuring the effects of structure formation imprinted upon the hot gas that is predicted to lie in extended halos around galaxies, groups, and clusters, (2) to determine how black holes influence their surroundings by tracing the propagation of out-flowing mass, energy and momentum from the vicinity of the black hole out to large scales and (3) to understand how accretion forms and evolves stars and circumstellar disks by observing hot infalling and out owing gas in these systems. *Arcus* relies upon grazing-incidence silicon pore X-ray optics with the same 12m focal length (achieved using an extendable optical bench) that will be used for the ESA Athena mission. The focused X-rays from these optics will then be diffracted by high-efficiency off-plane reflection gratings that have already been demonstrated on sub-orbital rocket flights, imaging the results with flight-proven CCD detectors and electronics. The power and telemetry requirements on the spacecraft are modest. The majority of mission operations will not be complex, as most observations will be long (~100 ksec), uninterrupted, and pre-planned, although there will be limited capabilities to observe targets of opportunity, such as tidal disruption events or supernovae with a 3-5 day turnaround. After the end of prime science, we plan to allow guest observations to maximize the science return to the community.



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TO MESS WITH AN ASTRONOMER, PUT A MIRROR IN THE PATH OF THEIR TELESCOPE.

https://xkcd.com/1231/

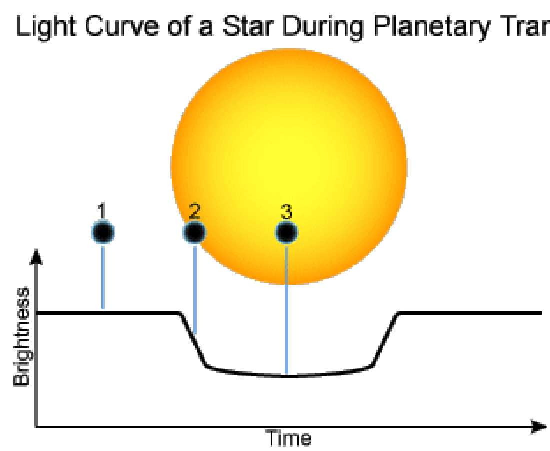
Exoplanets

A Survey Astronomy Laboratory Sequence Covering Exoplanets

Michael N. Fanelli

Abstract

The ongoing explosion of exoplanet discoveries since 1995 has created a new branch of astronomy, simultaneously scrambling the long-standing pedagogy for college-level astronomy courses. The universe of extrasolar planetary discussion topics does not fit easily into either the "Solar System" (Astro 101) or 'Stars & Galaxies "(Astro 102) courses. In addition to adjusting course content, new laboratory exercises are required, covering concepts like exoplanet detection methods, habitability and planetary properties. I have developed a set of laboratories, at the survey astronomy level, suitable for both Astro 101 & 102. These labs are organized around the theme "Architecture of Planetary Systems, Ours and Theirs". In this presentation I will describe the philosophy of the lab sequence, individual labs and some of the excellent online tools utilized. The entire sequence was developed and delivered to survey astronomy students at Foothill College and should be useful to those teaching similar classes.



Computing highly accurate spectroscopic line lists for characterization of exoplanet atmospheres and assignment of astronomical observations

Timothy J. Lee[a], **Xinchuan Huang**[a,b], **and David W. Schwenke**[c]
[a]Space Science & Astrobiology Division, NASA Ames Res. Ctr., Moffett Field, CA, USA
[b]SETI Institute, Mountain View CA, USA
[c]NAS Facility, NASA Ames Research Center, Moffett Field, CA, USA

Over the last decade, it has become apparent that the most effective approach for determining highly accurate rotational and rovibrational line lists for molecules of interest in planetary atmospheres and other astrophysical environments is through a combination of high-resolution laboratory experiments coupled with state-of-the art *ab initio* quantum chemistry methods. The approach involves computing the most accurate potential energy surface (PES) possible using state-of-the art electronic structure methods, followed by computing rotational and rovibrational energy levels using an exact variational method to solve the nuclear Schrödinger equation. Then, reliable experimental data from high-resolution experiments is used to refine the *ab initio* PES in order to improve the accuracy of the computed energy levels and transition energies. From the refinement step, we have been able to achieve an accuracy of approximately σ_{RMS}= 0.02 cm^{-1} for rovibrational transition energies, and even better for purely rotational transitions. This combined "experiment + theory" approach allows for determination of essentially a complete line list, with hundreds of millions of transitions, and having the transition energies and intensities be highly accurate. Our group has successfully applied this approach to determine highly accurate line lists for NH_3 and CO_2 (and isotopologues), and very recently for SO_2 and isotopologues. Here I will report our latest results for SO_2 isotopologues and updates on CO_2 isotopologues. Comparisons to the available data in HITRAN2016 and other available experimental data will be shown, though we note that our line lists for SO_2 isotopologues are significantly more complete than any other databases. Since it is important to span a large temperature range in order to model the spectral signature of exoplanets, we will also demonstrate how the spectra of CO_2 change on going from low temperatures (100 K) to higher temperatures (500 K to 1500 K).

Limits On Undetected Planets in the Six Transiting Planets Kepler-11 System

J. Lissauer, D. Jontof-Hutter, B. Weaver, E. Ford, D. Fabrycky

The Kepler-11 has five inner planets ranging from ~ 2 - 10 times as massive Earth in a tightly-packed configuration, with orbital periods between 10 and 47 days. A sixth planet, Kepler-11 g, with a period of 118 days, is also observed. The spacing between planets Kepler-11 f and Kepler-11 g is wide enough to allow room for a planet to orbit stabily between them. We compare six and seven planet fits to measured transit timing variations (TTVs) of the six known planets. We find that in most cases an additional planet between Kepler-11 f and Kepler-11 g degrades rather than enhances the fit to the TTV data, and where the fit is improved, the improvement provides no significant evidence of a planet between Kepler-11 f and Kepler-11 g. This implies that any planet in this region must be low in mass. We also provide constraints on undiscovered planets orbiting exterior to Kepler-11 g.

Using Final Kepler Catalog Completeness and Reliability Products in Exoplanet Occurrence Rate Estimates

Steve Bryson, Chris Burke, Natalie Batalha, Susan Thompson, Jeff Coughlin, Jessie Christiansen, Fergal Mullally, Megan Shabram

Burke et. al. 2015 presented an exoplanet occurrence rate estimate based on the Q1-Q16 Kepler Planet Candidate catalog. That catalog featured uniform planet candidate vetting and analytic approximations to the detection completeness (the fraction of true planets that would be detected) for each target star. We present an extension of that occurrence rate work using the final DR25 Kepler Planet Candidate catalog products, which uses higher-accuracy detection completeness data for each target star, and adds estimates of vetting completeness (the fraction of detected true planets correctly identified as planet candidates) and vetting reliability (the fraction of planet candidates that are true planets). These completeness and reliability products are based on synthetic manipulations of Kepler data, including transit injection, data scrambling, and inversion. We describe how each component is incorporated into the occurrence rate estimate, and how they impact the occurrence rate estimate both individually and in combination. Using these products in both the method of Burke et. al. 2015 and the inverse detection efficiency method, we find that the occurrence rate for planets between 1 and 2 Earth radii and orbital periods of 50-200 days is ~0.16 +- 0.02, about half the Burke et. al. 2015 baseline of 0.34. We discuss the strengths and weaknesses of the completeness and reliability products and how they impact our confidence in the occurrence rate values uncertainties. This work is an example of how the community can use the DR25 completeness and reliability products, which are publicly available at the NASA Exoplanet Archive (http://exoplanetarchive.ipac.caltech.edu) and the Mikulski Archive for Space Telescopes (http://archive.stsci.edu/kepler).

The Transiting Exoplanet Community Early Release Science Program for JWST

Batalha, Natalie M.; Stevenson, Kevin; Bean, Jacob; Sing, David; Berta-Thompson, Zach; Crossfield, Ian; Knutson, Heather; Line, Michael; Kreidberg, Laura; Desert, Jean-Michel; Wakeford, Hannah R.; Crouzet, Nicolas; Moses, Julianne; Benneke, Björn; Kempton, Eliza; Lopez-Morales, Mercedes; Parmentier, Vivien; Gibson, Neale; Schlawin, Everett; Fraine, Jonathan; Kendrew, Sarah; Greene, Tom; and 82 members of the *Transiting Exoplanet Community ERS Team*

The James Webb Space Telescope offers astronomers the opportunity to observe the composition, structure, and dynamics of transiting exoplanet atmospheres with unprecedented detail. However, such observations require very precise time-series spectroscopic monitoring of bright stars and present unique technical challenges. The Transiting Exoplanet Community Early Release Science Program for JWST aims to help the community understand and overcome these technical challenges as early in the mission as possible, and to enable exciting scientific discoveries through the creation of public exoplanet atmosphere datasets. With observations of three hot Jupiters spanning a range of host star brightnesses, this program will exercise time-series modes with all four JWST instruments and cover a full suite of transiting planet characterization geometries (transits, eclipses, and phase curves). We designed the observational strategy through an open and transparent community effort, with contributions from an international collaboration of over 100 experts in exoplanet observations, theory, and instrumentation. Community engagement with the project will be centered around open Data Challenge activities using both simulated and real ERS data, for exoplanet scientists to cross-validate and improve their analysis tools and theoretical models. Recognizing that the scientific utility of JWST will be determined not only by its hardware and software but also by the community of people who use it, we take an intentional approach toward crafting an inclusive collaboration and encourage new participants to join our efforts.

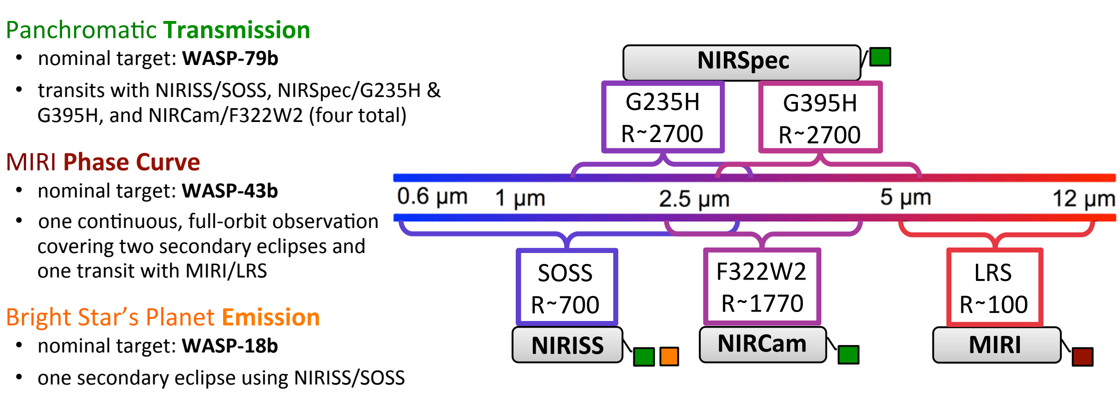


Figure 1 Three observing campaigns comprise the JWST ERS observing program for the transiting exoplanet community.

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https://xkcd.com/1752/

Aeolus: A mission to study the winds and climate of Mars.

A. M. Cook, A. Colaprete, Khare, M., Haberle, R.

Aeolus is a mission to directly measure the winds and climate of Mars, by measuring surface and atmospheric temperatures, aerosol abundances, and Doppler shifts in atmospheric spectral lines. The Planetary Science Division's (PSD) Science Plan includes goals to "explore and observe the objects in the Solar System to understand how they formed and evolved" and to "advance the understanding of how the chemical and physical processes in our solar system operate, interact, and evolve." Aeolus studies of the Martian atmosphere are derived from these NASA goals. Aeolus objectives are to: (1) Characterize Mars global circulation processes, including seasonal and diurnal changes, (2) determine the relative contributions to the global energy balance at Mars by measuring rejected solar radiation, and thermal emission from the Martian surface and atmosphere, and (3) measure Martian atmospheric aerosol (H_2O ice, dust) distribution.

To date, direct measurements of Martian wind speeds have only been possible at the surface, often only during daylight hours, and over small areas limited by rover traverse capabilities. From orbit, thermal measurements as well as images of dust storms and dune migration have provided inputs to derive the current state-of-the-art data sets in Mars climate modeling. However, Mars Global Circulation Models (GCM), like the one supported by the NASA Mars Climate Center at Ames Research Center, demonstrate that wind speeds derived from these indirect measurements may be more than 100% in error. For this reason, direct wind velocity measurements have been deemed "High Priority" by the Mars Exploration Program Analysis Group (MEPAG); measuring wind speeds and corresponding thermal data are vital to understanding Mars' climate. Notably, collecting data on Martian weather is paramount for planning landed and crewed missions at the surface. The measurements proposed for Aeolus will form the first set of global, seasonal, and diurnal data to characterize winds, which have a large influence on launch and landing constraints. The mission concept for Aeolus consists of a single spacecraft in a near-polar orbit, allowing it to pass over all local times, with near-global coverage of the surface. Aeolus mission duration is 2 Earth years, equivalent to 1 Mars year, in order to capture climate patterns during each Martian season.

The Aeolus concept first came about as a response to a new type of miniaturized Spatial Heterodyne Spectrometer (SHS), which could make wind measurements at Mars more affordable due to reduced instrument mass and thermal stability. The Aeolus spacecraft includes a system of four of these miniaturized SHS modules paired to two orthogonal viewing telescopes. This high-resolution near-infrared system can measure CO_2 (daytime absorption) and O_2 (day and night emission) lines in the Martian atmosphere. Doppler shifts in these lines, associated with winds speeds as low as 5 m/s, can be measured during Martian day and night. Identical modules are optically connected to one telescope each, so that each spectral line is observed with two orthogonal views as the spacecraft proceeds through its orbit. This allows line-of-sight wind speeds to be converted to wind vectors during ground processing.

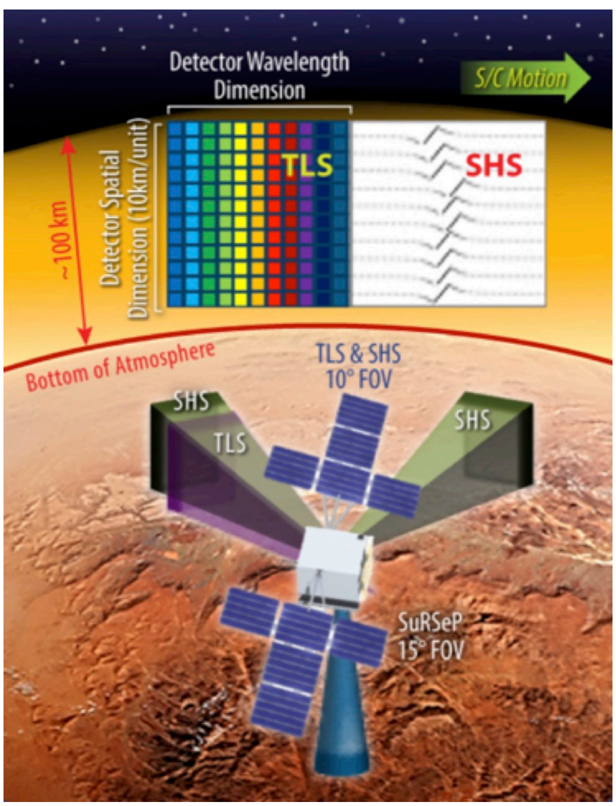


Figure 1. The combined fields of view for all three of the instruments in the Aeolus science payload.

Aeolus also has the Thermal Limb Sounder (TLS) instrument to measure atmospheric temperature profiles and aerosol (H_2O ice clouds, dust) profiles. Finally, the Surface Radiometric Sensor Package (SuRSeP) will measure the total reflected solar radiance, and surface temperatures down to 140K and total water ice cloud and dust column densities. Figure 1 shows a schematic of how each instrument views the atmosphere (Martian limb) or surface. Together, these combined spectral and thermal measurements will provide a new understanding of the global energy balance, dust transport processes, and climate cycles in the Martian atmosphere. Combining direct wind observations and simultaneous observations of the atmospheric drivers that force these winds, Aeolus provides a unique data set to understand Martian circulation and validate Mars climate models. These data will also constrain the design space for future missions that fly or float in the atmosphere, descend through the atmosphere, or land and operate on its surface.

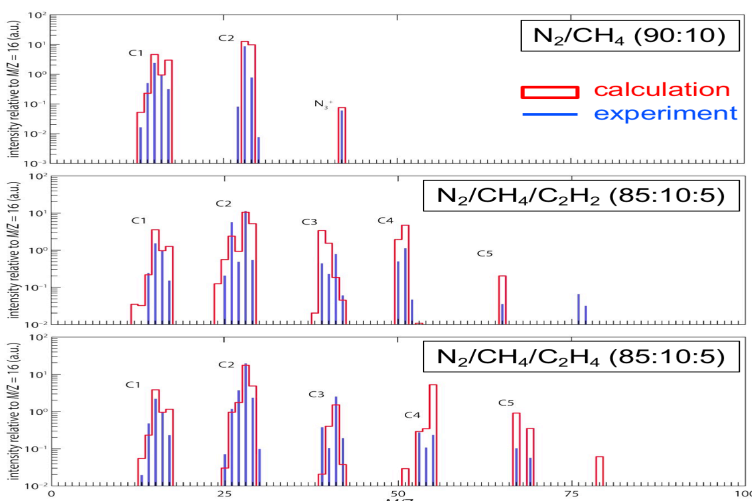
The Titan Haze Simulation Experiment: Dedicated Plasma Chemistry Model and Latest Laboratory Results

Sciamma-O'Brien E.[1, 2], Raymond A. W.[3], Upton K. T.[4], Mazur E.[3], Salama F.[1]
[1]NASA Ames Research Center, Moffett Field, CA, USA,[2]Bay Area Environmental Research Institute, Moffett Field, CA, USA [3]Harvard University, Cambridge, MA, USA, [4]Indiana University Bloomington, IN, USA

The Titan Haze Simulation (THS) experiment, developed at the NASA Ames COSmIC simulation chamber is a unique experimental platform that allows us to simulate Titan's complex atmospheric chemistry at Titan-like temperature (200 K) by cooling down N_2-CH_4-based mixtures in a supersonic expansion before inducing the chemistry by plasma. Both the gas and solid phase can be characterized.

Because of the accelerated gas flow in the expansion, the residence time of the gas in the active plasma region is less than 4 µs. This results in a truncated chemistry that enables us to control how far in the chain of chemical reactions the chemistry is processing, by adding, in the initial gas mixture, heavier molecules that have been detected as trace elements on Titan (Sciamma-O'Brien et al., 2014). This unique aspect of the THS has been confirmed by a new model developed to simulate the plasma chemistry in the THS, and which follows the evolution in time and space of more than 120 species using electron impact and chemical kinetics equations. The calculated mass spectra are in good agreement with the experimental THS mass spectra, confirming that the short residence time in the plasma cavity limits the growth of larger species (Raymond et al., 2018).

The THS solid phase component has also been characterized using scanning electron microscopy, infrared spectroscopy and x-ray absorption spectroscopy that have shown differences in the morphology of the grains produced as well as differences in the level and nature of the nitrogen incorporation depending on the composition of the initial gas mixture. A comparison to Cassini VIMS observational data has shown that the THS aerosols produced in simpler mixtures, i.e., that contain more nitrogen and where the N-incorporation is in isocyanide-type molecules instead of nitriles, are more representative of Titan's aerosols (Sciamma-O'Brien et al., 2017). In the next step in the analysis of the THS aerosols, a study will be initiated to determine their optical constants from the UV to the Far IR using a new optical constant facility that has recently been added.



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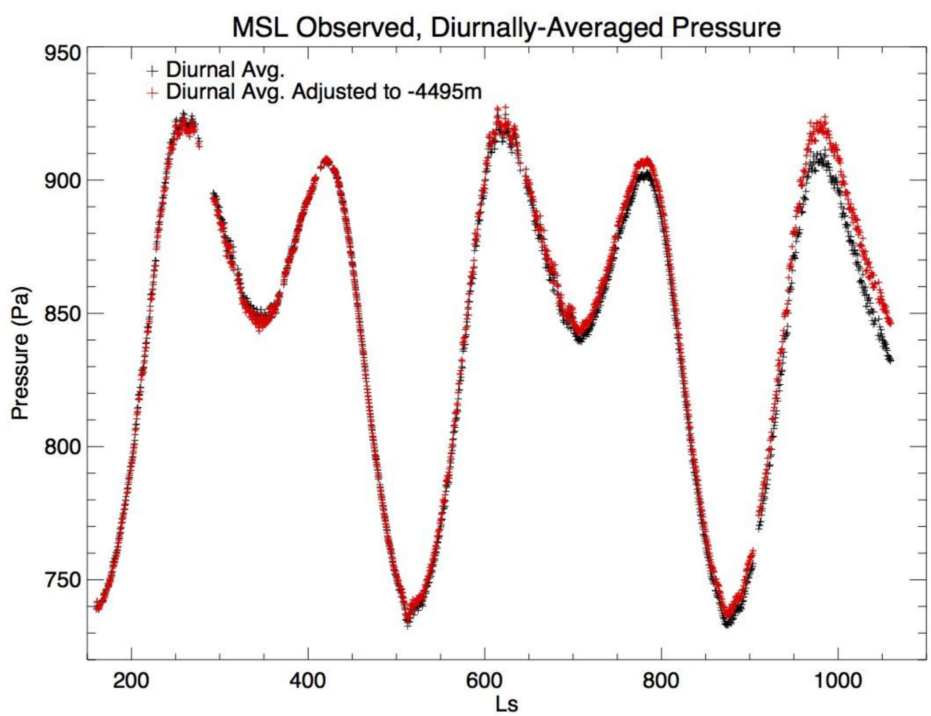
Acknowledgements: This research is supported by the SSW Program of NASA SMD and a SERA. The authors acknowledge the technical support of E. Quigley.

Detecting Secular Climate Change on Mars: An Update

Courtney M.L. Batterson[1,2], Melinda A. Kahre[2], Robert M. Haberle[2], R. John Wilson[2], and Henrik Kahanpää[3]
(1)Bay Area Environmental Research Institute, Petaluma, CA, USA, (2)NASA Ames Research Center, Moffett Field, CA, USA, (3)Finnish Meteorological Institute, Helinski, Finland

The stability of the South Polar Residual Cap (SPRC) has been in question since Leighton & Murray (1966) discovered the ice was made of primarily CO_2 in solid-vapor equilibrium with the atmosphere. In 2001, Malin et al. reported a net loss of cap mass that Blackburn et al. (2010) calculated would sublime the SPRC by the end of the decade. Also in 2010, Haberle & Kahre analyzed Phoenix and Viking Lander 2 (VL2) surface pressure data to quantify the net gain of atmospheric CO_2 since the time of the Viking Missions. Though their estimates were consistent with Malin et al. (2001), the accuracy of the Phoenix pressure sensor and its limited dataset rendered their study inconclusive. Our study quantifies the change in atmospheric mass since VL2 using data from the Curiosity rover, which has a stable pressure sensor of known accuracy and has recorded over two complete Mars Years of data. The difference in the annual mean surface pressure during the VL2 and MSL missions is calculated after accounting for the Curiosity pressure sensor warm-up time, rover elevation changes, diurnal bias, and missing data. Additionally, an ensemble of climate simulations from two Mars Global Climate Models (MGCMs) are used to define an offset that accounts for dynamical and physical differences between lander locations. Though the Legacy MGCM runs at fairly coarse horizontal resolution, our new higher-resolution MGCM that utilizes the NOAA/GFDL finite volume dynamical core is capable of resolving Gale Crater and its circulations. Our calculations estimate an atmospheric loss rate of ~5 Pascals per Mars Decade, which is comparable to the year-2 MSL sensor accuracy (~4 Pa). Coupled with the uncertain accuracy of the VL2 pressure sensor, we see no compelling evidence for secular climate change. This result is consistent with recent refinements in actual cap loss rates (see Thomas et al. 2016, Byrne et al. 2015, Becerra et al. 2015).

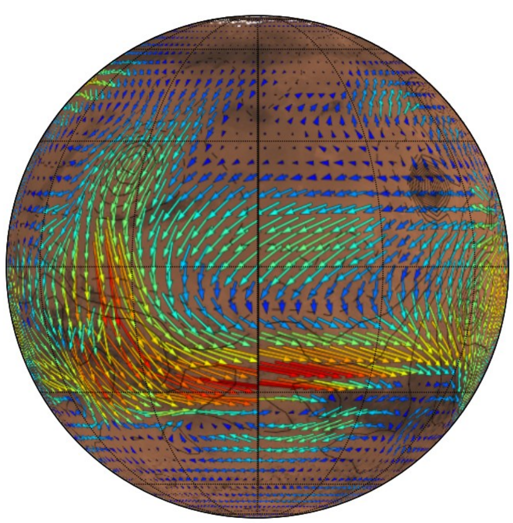


Investigating the closure of the dust cycle on current Mars by implementing the tagging method in the NASA Ames MGCM

T. Bertrand, M. Kahre, J. Wilson, A., Kling

National Aeronautics and Space Administration (NASA), Ames Research Center, Space Science Division, Moffett Field, CA 94035, United States

Climate science is at the heart of many issues and challenges of this century. Studying other planets enables us to increase our understanding of climate processes. Investigating Mars, which is the objective of many space missions, is particularly illuminating. The climate of Mars is characterized by complex interactions between CO_2, water, and dust cycles, as revealed by the different orbiters, landers and rovers. Many fundamentally issues remain unsolved regarding the current climate of Mars, and the dust and water cycles in particular. Our project seeks to provide new insights on the following overarching questions: *What are the role and impact of the reservoirs of dust and water on the cycles? What controls and triggers the regional and global dust storms? Where and how is dust lifted and transported in the atmosphere?* We aim to answer these questions by providing a new global vision of the dust cycle on Mars by implementing the so-called tagging method in the NASA Ames Mars Global Climate Model (MGCM). The tagging method consists in “tagging” or “labeling” the transported constituents of the atmosphere according to a chosen criterion. As an example, dust particles could be the tagged constituent (« dust tagging ») and the criterion its geographic origin (e.g., the Hellas Planitia basin). This means that during the entire simulation, we keep track of the dust particles that originate in the selected regions of Mars. This approach, never tested before on Mars, has plenty of promising applications. It enables us to investigate the closure (or non-closure) of the current dust cycle, quantify the exchanges between the different dust sources and sinks in the present-day climate system, and determine the long-term mass balance and equilibrium state of the dust cycle. In particular, we can assess the impact of finite surface dust reservoirs, radiatively active clouds and scavenging by water ice clouds on the dust lifting, transport and deposition, and use the results and high resolution modeling to better understand dust storms generation. We will present preliminary results showing how dust exchanges between the main surface and atmospheric reservoirs.



The Latest on the Venus Thermospheric General Circulation Model: Capabilities and Simulations

Amanda Brecht[1], S. W. Bougher[2], C. D. Parkinson[2]

[1] *NASA Ames Research Center, M/S 245-3, Moffett Field, CA, 94035, USA;*
[2]*CLaSP, 2418C Space Research Building, University of Michigan, Ann Arbor, MI, 48109, USA*

Abstract: Venus has a complex and dynamic upper atmosphere. This has been observed many times by ground-based, orbiters, probes, and fly-by missions going to other planets. Two over-arching questions are generally asked when examining the Venus upper atmosphere: (1) what creates the complex structure in the atmosphere, and (2) what drives the varying dynamics. A great way to interpret and connect observations to address these questions utilizes numerical modeling; and in the case of the middle and upper atmosphere (above the cloud tops), a 3D hydrodynamic numerical model called the Venus Thermospheric General Circulation Model (VTGCM) can be used. The VTGCM can produce climatological averages of key features in comparison to observations (i.e. nightside temperature, O_2 IR nightglow emission). More recently, the VTGCM has been expanded to include new chemical constituents and airglow emissions, as well as new parameterizations to address waves and their impact on the varying global circulation and corresponding airglow distributions. These improvements to the VTGCM enable the model to address the driving forces in Venus' upper atmosphere and its' variability.

Chemistry: The SOx chemistry has been included (e.g. SO_2 and SO) and also the necessary OH chemistry to model the OH nightglow emission. The inclusion of these chemical species (and nightglow emission) provides tracers of the global circulation at different altitudes in the upper atmosphere.

Aerosol Heating: The VTGCM lower boundary is at ~70 km, which is near the cloud tops. Near this level, aerosols provide heat to the middle atmosphere. A parameterization has been incorporated and tested. The additional heating increases the scale heights in this altitude range (~75-90 km) and therefore augments density profiles (~100-130 km) and modifies wave propagation.

15 μm Cooling Parameterization: A simplified non-LTE formulation utilized within LMD-MGCM and LMD-VGCM is being imported into the VTGCM. The non-LTE model uses five CO_2 levels and bands, instead of two molecular levels. It calculates the full exchange between atmospheric layers, instead of using the cool-to-space approximation which was the basis of the previous parameterization in the VTGCM. We expect to find VTGCM temperatures warmer over ~80-110 km (day and night) and about the same (cool to space approximation is fine) in the Venus dayside and nightside thermosphere (above ~110-120 km).

Planetary Waves: Due to observations of waves near the cloud tops, Kelvin and Rossby planetary waves have been implemented as part of the VTGCM lower boundary. But most importantly, they have been implemented with a self-consistent moving lower boundary (winds are not equal to zero and temperature is not constant). This lower boundary is taken from the Oxford Venus GCM; 5 day time averaged fields (T, U, V, Z) are utilized. The combination of the moving lower boundary and Kelvin waves produces variability which impacts the intensity and local time location of the O_2 IR nightglow emission. These variations in the nightglow emission (as much as ~1-3 MR) are of a similar magnitude as observations. Waves are important to understand because of their impact on the varying dynamics of Venus' upper atmosphere.

The work to be presented will include a reference VTGCM simulation showing the impacts the latest improvements make upon the upper atmosphere and how the results compare to observations. Also, the utility of the VTGCM with respect to future mission (Venera-D) will be described. The comparative work relating modeling and observations is very important to improving our understanding of the underlying processes driving the complex and dynamical structure of the upper atmosphere of Venus.

Title: Maintenance of background dust opacity with wind stress based dust lifting during northern hemisphere summer on Mars.

Authors: Vandana Jha and Melinda Kahre

Introduction: The Martian atmosphere contains dust throughout the year but the atmospheric dust load varies with season. A background haze of atmospheric dust is maintained throughout northern hemisphere spring and summer and the dust activity is heightened during southern spring and summer. In the absence of regional or global storms, dust devils and local storms maintain the background dust loading during the non-dusty season. Mars Global Surveyor (MGS) Mars Orbiter Camera (MOC) observations indicate that small regional dust events persist throughout northern spring and summer. Observational surveys of dust devils and general circulation modeling results suggest that it is likely that dust devils are responsible for the presence of atmospheric dust during these seasons. However, a quantitative understanding of the relative contribution of dust devils and local dust storms has not yet been achieved. Here we present preliminary results from an investigation that focuses on the effects of radiatively active water ice clouds on dust lifting processes. Radiatively active water ice clouds influence the thermal structure of the Martian atmosphere and can thus affect dust lifting through radiative-dynamic feedbacks.

Methods: The primary tool for this work, the NASA Ames Legacy MGCM, is a 3 dimensional model that has been used for investigations of the past and current climate of Mars. A horizontal resolution of 5° in latitude and 6° in longitude is used for the study.

Experimental Simulations: Three simulations that included wind stress dust lifting were executed for a period of 5 Martian years: a case that included no cloud formation, a case that included radiatively inert cloud formation, and a case that included radiatively active cloud (RAC) formation. Water ice clouds are known to affect atmospheric temperatures directly by absorption and emission of thermal infrared radiation. They also affect the temperatures indirectly through dynamical feedbacks. The aphelion cloud belt and the polar hood clouds are two prominently observed types of clouds. The aphelion cloud belt is composed of optically thin clouds that form above 10-15 km at low latitudes during northern spring and summer (L_s~50-135°. Polar hood clouds are optically thick and may or may not extend down to the surface.

Results: Figure 1 shows a comparison of the globally averaged wind stress dust lifting rates for all three simulations during NH spring and summer. It is evident that the inclusion of radiatively active clouds in the simulation enhances the global dust lifting rates by approximately an order of magnitude. This enhancement is the result of radiative/dynamic feedbacks due to water ice clouds. Radiative heating by clouds in the aphelion cloud belt warms the atmosphere aloft at low latitudes while low-lying polar clouds radiatively cool the low-level polar atmosphere. This increased equator-to-pole thermal gradient drives an enhanced overturning circulation. The stronger overturning circulation produces an enhanced low-level flow in the Hadley cell return branch, which in turn produces higher surface stresses and increased dust lifting in those locations.

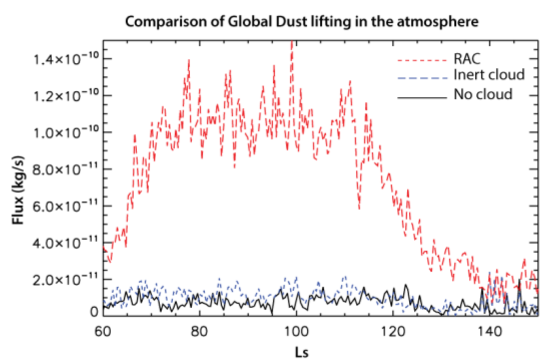


Figure 1: Globally averaged dust lifting rates for simulations without clouds, with radiatively inert clouds, and with radiatively active clouds.

Conclusions: Our results suggest that with radiatively active clouds included, radiative-dynamic feedbacks generate a stronger mean overturning circulation and more pronounced wind stress dust lifting and a slightly higher overall dust loading during NH spring and summer. These results suggest that wind stress lifting may contribute more to maintaining the background dust haze during NH spring and summer than what previous studies have shown. However, dust devils are still important for maintaining the background haze in the atmosphere during that time of the year.

Title: Recent Advances in Simulating the Martian Climate with the NASA Ames Mars Global Climate Model

Authors: Melinda A. Kahre, Jeffery L. Hollingsworth, R. John Wilson, Robert M. Haberle, Amanda S. Brecht, Richard A. Urata, Alex Kling, Vandana Jha, Courtney M. Batterson, Tanguy Bertrand, and Kathryn E. Steakley

NASA's Mars Climate Modeling Center at Ames Research Center is currently undergoing an exciting period of growth in personnel, modeling capabilities, and science productivity. We are transitioning from our legacy C-grid finite-difference dynamical core to the NOAA/GFDL cubed-sphere finite-volume (FV3) dynamical core for simulating the climate of Mars (Figure 1). This highly parallelized core is scalable and flexible, which will allow for significant improvements in the horizontal resolution of our simulations. We are currently porting the Mars-specific physical process codes developed here at Ames over the past several decades into the new dynamical core. In addition to this new model development, our group has made progress advancing our understanding of the current and past climate of Mars. We have addressed many questions regarding the current CO_2, dust and water cycles and the dynamical processes that control them. Further, we have begun investigations into the photochemistry and transport processes of the upper atmosphere. Finally, we have initiated studies of the climate systems of the Amazonian, Hesperian, and Noachian periods of Martian history. We will present these new model capabilities and insights into the atmosphere and climate of Mars.

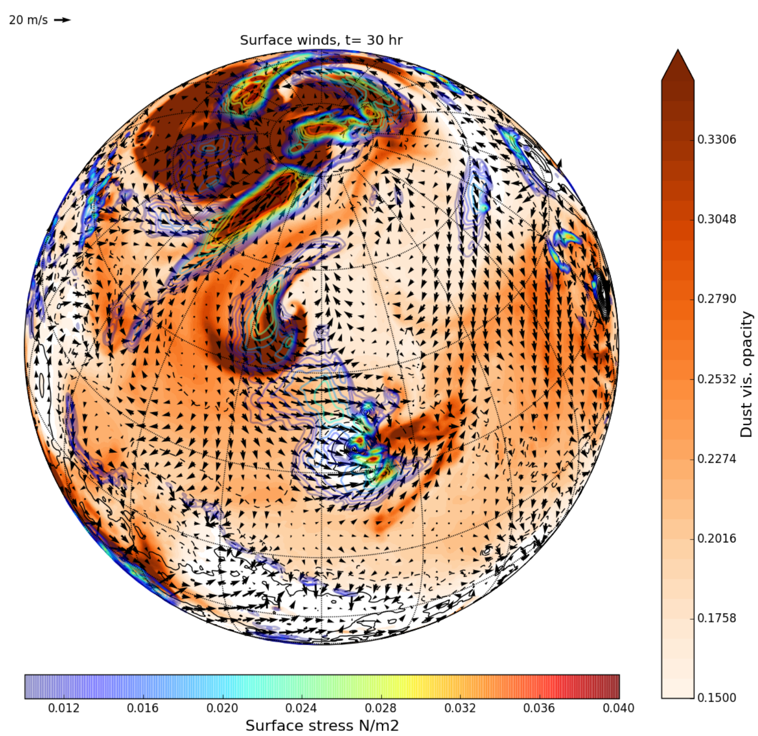


Figure 1: Column dust opacity (shading), surface wind stress (contours) and low-level winds (vectors) from a high-resolution simulation with the NASA Ames Mars GCM that features a new dynamical core. Wind vectors are subsampled for clarity. These instantaneous fields are from an animation used to explore interactions between dust lifting, dust transport, and the general circulation.

Title: Modularization in the Ames Mars General Circulation Model Ecosystem

Authors: Richard A. Urata, Melinda A. Kahre, John Wilson, Jeffery L. Hollingsworth

Abstract:

The Ames Mars general circulation model (MGCM) currently in use has a long lineage dating back to the first 1 dimensional model described by Pollack et al. (1976). The latest version of the model employs an Arakawa C-grid for dynamical calculations, and advanced physics developed for the Martian climate including among others, a boundary layer scheme based off of level-2 Mellor-Yamada turbulence closure, a two-stream k-coefficient radiative transfer scheme, and a two-moment microphysics scheme for dust and ice. There is an issue with the Arakawa C-grid however, that the meridians converge at the poles meaning that it becomes increasingly difficult to satisfy the CFL condition, especially with finer model horizontal resolution. Luckily for us, the terrestrial modeling community has significantly more resources devoted to development, and have come up with a number of ingenious solutions to this very problem. The GFDL terrestrial model (FV3) for example, uses a finite-volume "cubed-sphere" grid made up of six square tiles that are sewn together at the edges to make a sphere.

In an effort to modernize the Ames MGCM, we aim to utilize these new modeling frameworks such as FV3, while retaining as much of the sophisticated physics developed for the Ames MGCM. In an ideal world, we would perform basic comparisons between multiple different modeling frameworks using the same physics in order to determine the effects of the numerical grid. To reach this goal, it is important to make the implementation of the Mars physics packages as simple as possible, which leads to the concept of modularization. With modular physics, anyone would be able to implement any modularized part of the Ames Mars physics with a few simple modifications. This effort will greatly smooth the current as well as any future transitions of the Ames MGCM to a more modern framework, and allow for other Mars modeling efforts to take advantage of the advancements made by the Mars Climate Modeling Center with ease.

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ASSESSING ATMOSPHERIC THERMAL FORCING FROM SURFACE PRESSURE DATA: SEPARATING THERMAL TIDES AND LOCAL TOPOGRAPHIC INFLUENCE

R. J. Wilson, *NASA Ames Research Center (Robert.J.Wilson@nasa.gov),* **J. M. Murphy,** *New Mexico State University, Las Cruces, USA.*, **D. Tyler**, *Oregon State University, Corvallis, OR, USA.*

The evolving distribution of radiatively active dust and water ice clouds plays a major role in modulating the seasonal and interannual variation in the thermal forcing of the Martian atmosphere, and thus the resulting intensity of the circulation. Thermal tides are the global-scale atmospheric response to the diurnally varying thermal forcing, due to aerosol heating within the atmosphere and radiative and convective heat transfer from the surface. The global tide includes westward propagating (sun-synchronous) waves driven in response to solar heating, as well as nonmigrating waves that result from zonal variations in the thermotidal forcing that are caused by variations in the surface (the topography and surface thermal properties) and the distribution of aerosols (dust and water ice clouds). The migrating tides are of particular interest, since they tend to be directly responsive to the aerosol distribution. However, distinguishing these tides from the mix of additional nonmigrating tides is difficult with only a limited number of surface observations.

We utilize a very high resolution Mars Global Circulation Model to simulate diurnal variability at scales ranging from craters to the planetary scale, thus distinguishing the pressure signature of local topographically driven circulations from that of the global tide. We define the latter as that resulting from a reconstruction of surface pressure using a compact set of tide modes derived from a space-time analysis of suitably normalized simulated surface pressure. This field includes the migrating tides, resonantly enhanced Kelvin waves and a small set of additional nonmigrating tides. The remaining residual pressure field is found to be highly localized and clearly associated with smaller-scale topographic features (such as craters), while the thermal tide reflects the effect of forcing at planetary scales. With this approach, it is possible to isolate the influence of local topographic circulations on the diurnal variation of surface pressure. With this approach, it is possible to isolate the influence of local topographic circulations on the diurnal variation of surface pressure from that of the global thermal tide, thus enabling the comparison of surface pressure observations at lander sites with the global tide constructed from model results.

Maps of the amplitude of the diurnal harmonic of the residual pressure response are shown in Fig. 1. There is a clear association of early phase response (typically ~0400-0800 LT) within craters, channels, and basins, while the late phase response is seen in regions of elevated terrain adjacent to steep slopes. These late-phase instances are evidently due to the strong slope wind effects, as can be seen quite clearly near the peaks of the various steep volcanoes and in the highlands forming the western rims of Hellas basin and Isidis Planitia.

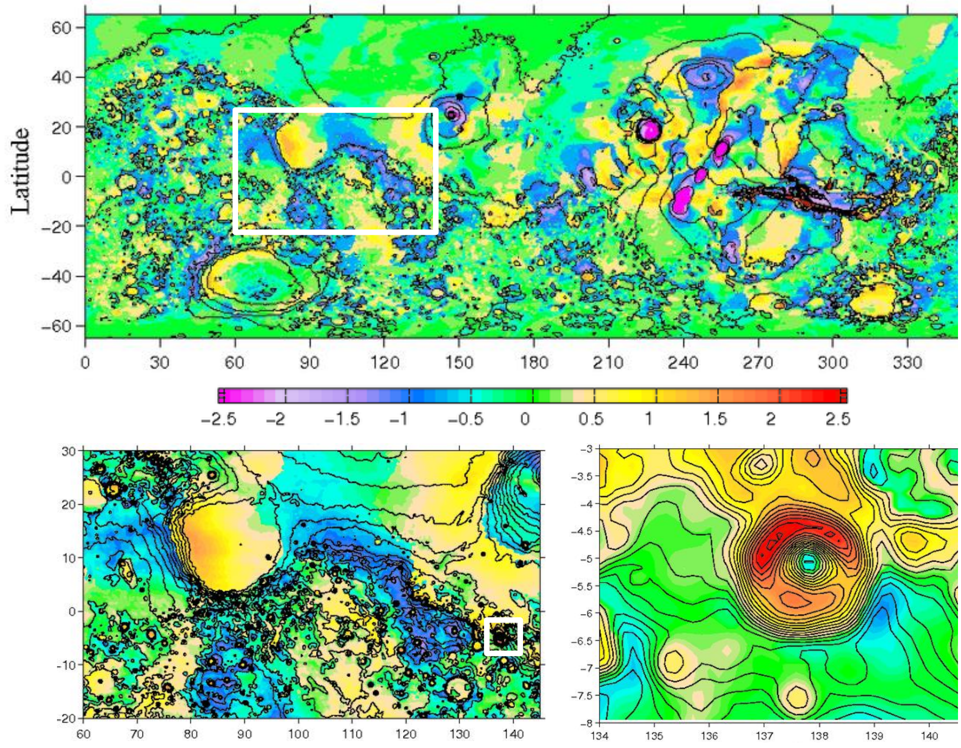

Figure 1 (a) The amplitude of the diurnal component of the residual pressure at L_s=188° as a percentage of the diurnal mean pressure. Positive values indicate regions where the phase is earlier than 1200 LT while negative values correspond to regions with the amplitude maximum after 1200 LT. Topography is contoured at intervals of 2 km. (b) Zoomed view of the residual pressure signal with topography shown at 0.5 km intervals. (c) A zoomed view of Gale crater with topography at 0.25 km intervals.

Beyond Mie Theory: Scattering by Spheroidal Particles

Sanford Davis

See poster or email Sanford.S.Davis@nasa.gov for abstract.

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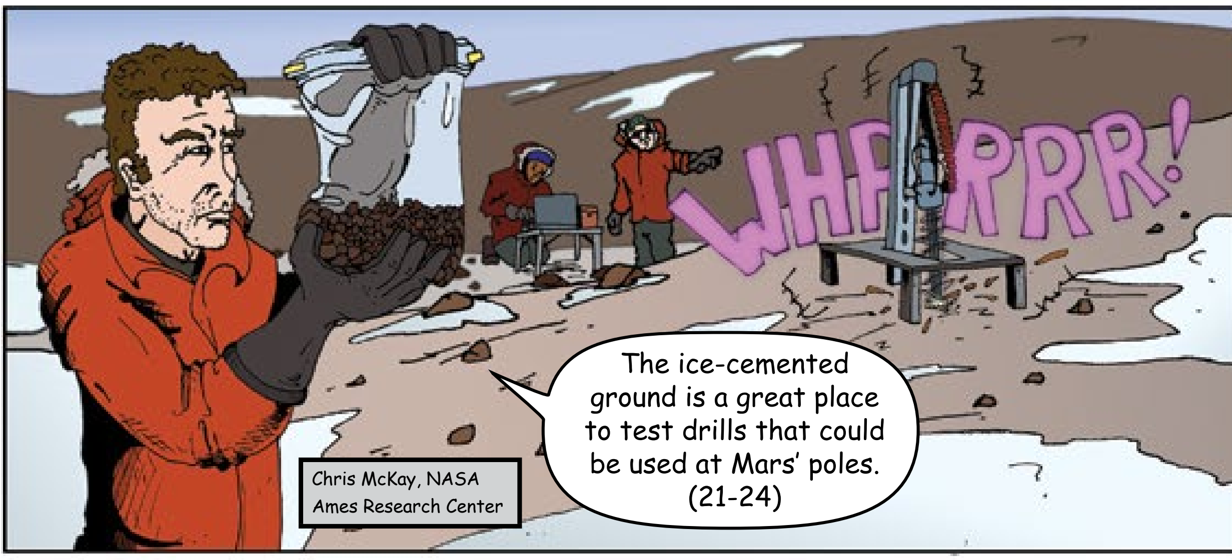

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Planetary Surfaces & Interiors

MICRO-CT ANALYSIS OF METEORITE FLAWS AND SCALING FOR ASTEROID ATMOSPHERIC ENTRY.
K. L. Bryson[1,2], D.R. Ostrowski[1,2], P. Agrawal[1,3], and F. Panerai[1,3], [1] NASA Ames Research Center, [2]BAER Institute, [3]Analytical Mechanics Associates, Inc. E-mail: kathryn.bryson@nasa.gov.

Introduction: Research is being conducted to understand the behavior of asteroids entering the atmosphere in order to help quantify their impact hazard. The strength of the body plays a critical role in determining the outcome of their impact events [1] and is needed for asteroid mitigation options. Meteorites are the material we have here to understand the larger parent body. Our objective is to scale flaw parameters in meteorites to their parent body, providing a way to scale strength from the meteorites to the asteroids.

Assuming that flaws follow the Weibull distribution [2], where flaws are assumed to be randomly distributed through the body and the likelihood of encountering a flaw increases with distance. The strength of the object can then be scaled based on the scaling factor called the Weibull coefficient, α. The value for α is unclear [3] and a large range has been determined from light curve data [1]. Very few measurements have been done through stress testing to determine α [4], due to the destructive nature of the technique.

Images of meteorites provide a 2D view of the flaws. A relationship exists between the distributions of measured trace length and actual flaw size [5]:

$$N_L=k_L L^{-1/(2\alpha)+1} \quad (1)$$

where N_L is the number per unit area of 2D flaw traces greater than length, L, and k_L is a constant. Therefore, the slope of a log-log plot of trace length versus flaw density is proportional to α.

Hand samples of meteorites have previously been used to determine a scaling factor [6,7]. This study is examining micro-CT measurements to understand the distribution of flaws throughout the entire sample.

Experimental: Micro-tomography (micro-CT) measurements of metorites with varying sample sizes were performed. The high metal content in the meteorites can create a lot of noise, making it harder to identify flaws in larger samples. The density and length of flaws were measured in selected slices from the stack of scans using ImageJ. For the smaller sample sizes with higher resolution we are able to use a ridge tracing plugin to measure the flaws, while in the larger samples the flaws were hand tranced.

Results and Discussion: Figure 1 plots the flaw length and denstities of a selection of slices from the mirco-CT scans of both a smaller fragment (blue) and larger fragment (red) of Tamdakht. A power law is fit to the a data, and an α of 0.162 ± 0.033 is detrermined. This is comparable to the commonly used value of 0.166 [8], but lower then the value previously determined for Tamdakht from hand sample and thin section images, 0.188 ± 0.025 [6], but is within the error. Some of this variation may be caused by the lack of resolution in the larger samples, making it hard to identify flaws. The value is less then value published based on stress testing of Tamdakht [5], 0.578 ± 0.0201. The cutting of samples during preparation for Cotto-Figueroa et al.'s 2016 stress testing did break several cubes biasing their test cubes, providing a more heterogeneous flaw distribution than was present through the original larger samples. This bias is likely causing the difference between our determined α.

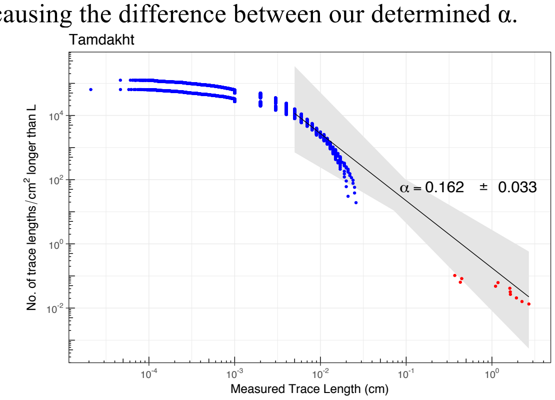

Figure 2. *Distribution of flaw trace length for Tamdakht based on a selection of slices of micro-CT scans. The blue points indicate measurements on the smaller fragment, while the red dots represent measurements from the larger fragment. The black line is the relationship between trace density and length, with a slope providing α, and the grey denotes the error.*

Conclusion: Initial analysis of length and density of flaws in a meteorite using selected slices from micro-CT scans indicates that it is possible to get a Weibull coefficient, α, within error of previously determined values based on hand and thin section analysis. Variations are observed from stress test values, but this is likely due to more heterogeneous samples being stress tested. Continued analysis of additional slices and samples will further validify this technique.

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Poster Title: Ammonia on Charon: Laboratory Optical Constants of Ammonia Hydrates to Support *New Horizons* Observations

Authors: Joseph Roser[1,2], Alessandra Ricca[1,2], Cristina Dalle Ore[1,2], and Dale Cruikshank[2]
Affiliations: (1) SETI Institute (2) NASA-Ames Research Center

Abstract: An absorption feature at 2.21 μm has been detected on Pluto's moons Charon, Nix, and Hydra, as well as the dwarf planet Orcus and possibly Quaoar. This feature is believed to be indicative of ammonia and/or ammonia hydrates being present on the surface layers of these bodies. In the case of Charon, this is unusual since Charon's radiation environment is expected to destroy ammonia and ammonia hydrates rapidly. The discovery of these feature on the very small bodies Nix and Hydra and the discovery that ammonia on Charon is isolated within ammonia-rich, bright-rayed craters suggest that a sub-surface reservoir of ammonia, not cryovolcanism, may ultimately be responsible for this surface component. In this view, the ammonia molecules in the shallow interior diffuse through the water ice that covers the satellite, acquiring a hydrate structure as it reaches the exposed surface. This can be seen as a continuing process as NH_3 is destroyed when exposed to solar ultraviolet light and is then replenished as more ammonia diffuses upward. Published laboratory studies support the conversion of NH_3 to $NH_3 \cdot nH_2O$ as it diffuses through pure H_2O ice.

To better understand the origin of this 2.21 μm feature, we have undertaken a combined program of laboratory experiments to be conducted at NASA-Ames Research Center to measure the optical constants of ammonia/water ice mixtures and ammonia hydrates in addition to quantum chemistry calculations for these systems. These data will be used in models of Charon's reflectance spectrum in order to better determine the specific ammonia ices present on Charon.

HIGH TEMPERATURE EMISSIVITY OF METEORITES RELATED TO ASTEROID ATMOSPHERIC ENTRY.
D. Ostrowski[1,2] and K. Bryson[1,2], [1]NASA Ames Research Center, Moffett Field, CA, USA., [2]Bay Area Environmental Research Institute, Ames Research Center, Moffett Field, CA, USA.

Introduction: Thermal properties are an important fundamental characteristic of the meteorites; an indicator of both their chemical and physical nature. Physical properties are needed to determine the likelihood of meteoroids survivability during atmospheric entry. Ablation models require the input of emissivity [1,2]. The Asteroid Threat Assessment Project has been set up to investigate the full risk and outcomes that near Earth asteroids pose to the planet.

Meteorites contain both high and low thermally conductive materials. Darkening material emissivity will increase as temperature increases until peak temperature is reached and then begins to decrease [4]. The metal components will slowly increase the emissivity as temperature increases, while the non-metallic material's emissivity will decrease.

Experimental: Thermal emissivity for the selected meteorites has been measured over a broad wavelength range of 8 to 14 µm from ~20°C up to 600°C. Emissivity values for up to atmospheric entry temperatures are needed for modeling. At elevated temperatures meteorites are heated in a nitrogen atmosphere to limit the effects of oxidation. Emissivity is measured by dual laser infrared thermometers. The ratio of the meteorite temperature to the blackbody temperature is calculated as the emissivity.

Results: Average emissivity of ordinary chondrite falls and Antarctic meteorites at 20°C is 0.988±0.008, in agreement with previously published values for ordinary chondrites [3]. For the howardite and eucrite finds the average emissivity is 0.997±0.03 at 20°C.

Increased temperature to 100°C the emissivity decreases then rebounds and stabilizes for the next 100° (Fig. 1). The largest change is observed between 20°C to 40°C, with the average emissivity droping 0.045. Nearly all chondrites heated to between 300/350°C have emissivities below 0.90. Heated chondrites range in emissivity between 0.85-0.95. When comparing values between ordinary chondrite falls and Antarctic meteorites no notable differences are observed.

Trends for NWA 2060 and NWA 7874 are similar to the ordinary chondrites. One sample of NWA 2060 does not follow the trend. Cube 1 of NWA 2060 emissivity drops slightly upon heating and broad u-shaped feature begins at 100°C and goes out to 180°C, having a higher emissivity than other basaltic meteorite. The variation in emissivity within NWA 2060 is likely due to its inhomogeneity. Continued heating results in all howardite and eucrite samples with emisivity values just below 0.90.

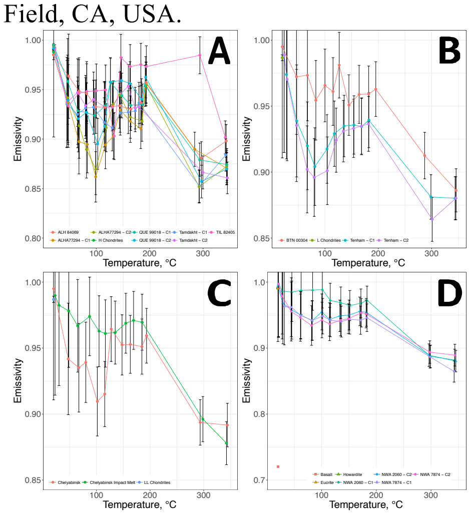

Figure 1. *Emissivity for low and intermediate temperature. Emissivity for H chondrites (A), L chondrites (B), LL chondrites (C), howardite and ecurite (D).*

Table 1. *High temperature emissivity measurements of at standard atmosphere and nitrogen atmosphere.*

Meteorite	Type	Temperature (°C)	Emissivity
Tamdakht	H	577.2	0.941±0.005
Tamdakht in Nitrogen	H	527.7	0.94±0.01
BTN 00304	L	578.0	0.904±0.004
TIL 820405	H	580.0	0.932±0.005

The heating of samples to near 600°C results in an increase in emissivity for ordinary chondrites (table 1) compared to measured values at 350°C. It appears that for Tamdakht, oxidation has no effect on the emissivity with the two different atmosphere samples having the same emissivity within error.

Conclusion: Thermal emissivity is a uniform trend across both falls and Antarctic finds. Meteorites show a broad decrease and rebound in emissivity below 200°C. The lowest emissivities are between 0.84 and 0.90 across all meteorite types. Decreasing emissivity at intermediate temperatures result in an increased rate of ablation for its parent meteoroid. Similar results are observed in ureilites [4]. Opposite trend is observed in the emissivity of chondrites at elevated temperatures. This implies H chondrite meteoroids will have a greater rate of energy transfer and thus lower ablation rates.

References: [1] Lyne et al. (1996) *JGR*, 101, 23,207-23,212. [2] Campbell-Brown M.D. et al. (2013) *A&A,* 557, A41, 1-13. [3] Baldridge A. M. et al. (2009) *Remote Sensing of Environment, 113,* 711-715. [4] Loehle S. et al. (2017) *M&PS*, 52, 197-205.

Using Satellite Data to Differentiate between Rock and Regolith on Earth's Surface

Corina Cerovski-Darriau and Jonathan Stock

USGS—Geology, Minerals, Energy and Geophysics (GMEG) Science Center—Menlo Park, CA

The distribution of soil is key to understanding water storage, carbon storage, cultivable land, natural hazard impacts (e.g. landslides) and other pertinent scientific, resource and safety questions both on Earth and beyond. Mapping regolith, or the mobile layer of material overlying bedrock, provides a distribution of soils in order to answer these questions. In particular, we are currently trying to determine where shallow, storm-driven landslides cannot occur for the state of California. Since steep slopes and soil cover is a prerequisite for slope failure, by mapping distribution of regolith versus exposed bedrock also creates a map of areas susceptible to landsliding. We are trying to determine the best dataset to differentiate between the two materials. ASTER hyperspectral data offer the ability to calculate apparent thermal inertia using albedo and daytime and nighttime temperatures. While this is successful at mapping bedrock, the spatial availability is lacking. Landsat offers the ability to attempt band math differencing to highlight various materials, but it not highly accurate statewide. We are still exploring additional potential datasets that provide sufficiently high resolution data and accurate differentiation between regolith and bedrock.

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